

# STIC Search Report Biotech-Chem Library

## STIC Database Tracking Number: 957

TO: Ganapathy Krishnan

Location: 8d08 / 8b19 Thursday, June 05, 2003

Art Unit: 1623 Phone: 305-4837

Serial Number: 10 / 009805

From: Jan Delaval

**Location: Biotech-Chem Library** 

CM1-1E07

Phone: 308-4498

jan.delaval@uspto.gov

### Search Notes

Jan Delaval Reference Librarian Biotochnology & Chemical Library CM1 1E07 - 703-308-4498 jan.delaval@uspto.gov



=> fil reg FILE 'REGISTRY' ENTERED AT 11:13:35 ON 05 JUN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JUN 2003 HIGHEST RN 525536-93-0 DICTIONARY FILE UPDATES: 4 JUN 2003 HIGHEST RN 525536-93-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d sta que 129 L5 STR

VAR G1=C/17/19/21/24/28/33/39 VAR G2=48/49NODE ATTRIBUTES: 49 NSPEC IS RC AT4 CONNECT IS M1 RC AT CONNECT IS M1 RC AT 13 RC AT 14 CONNECT IS M1 RC AT 40 CONNECT IS M1

RC AT

49

CONNECT IS M1

Jan Delaval
Reference Librarlan
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

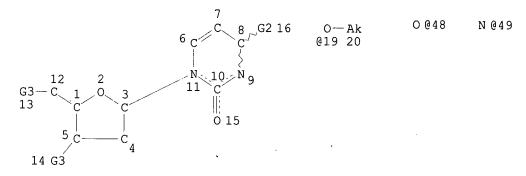
RSPEC 4 11

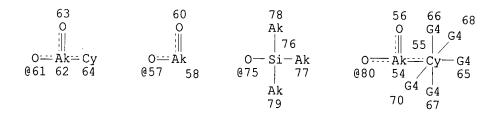
NUMBER OF NODES IS 47

STEREO ATTRIBUTES: NONE

L7 69658 SEA FILE=REGISTRY CSS FUL L5

L14 STR





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NODE ATTRIBUTES:
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CONNECT IS M1 RC AT 4
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 4 11

NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE L17 STR

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VAR G4=H/AK/X/19

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NSPEC IS RC AT 49 CONNECT IS M1 RC AT 7

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RSPEC 4 11

NUMBER OF NODES IS 45

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L21	5421	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L20/COM
L22		STR				

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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 4(

STEREO ATTRIBUTES: NONE

L23 5421 SEA FILE=REGISTRY SUB=L21 CSS FUL L22

STR

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 4

CONNECT IS M1 RC AT 7

CONNECT IS M1 RC AT 13

CONNECT IS M1 RC AT 14

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

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L27

SCR 2039 OR 2048 OR 2043 OR 2054 OR 2041 OR 2053

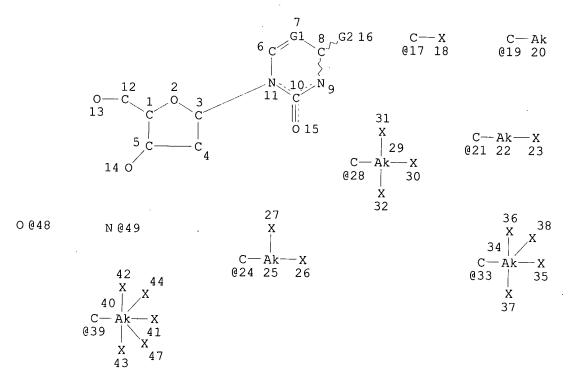
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100.0% PROCESSED 2046 ITERATIONS

2036 ANSWERS

SEARCH TIME: 00.00.01

=> d sta que 141 L5 STR



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DEFAULT ECLEVEL IS LIMITED

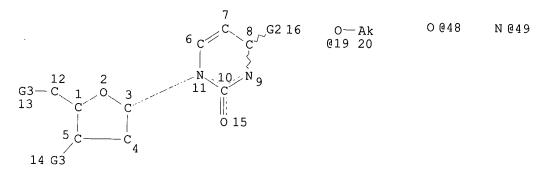
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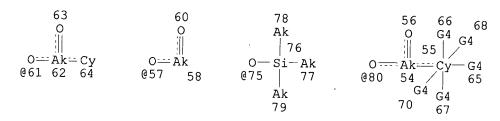
RSPEC 4 11

NUMBER OF NODES IS 47

STEREO ATTRIBUTES: NONE

L7 L14 69658 SEA FILE=REGISTRY CSS FUL L5 STR





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VAR G4=H/AK/X/19

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CONNECT IS M1 RC AT 7

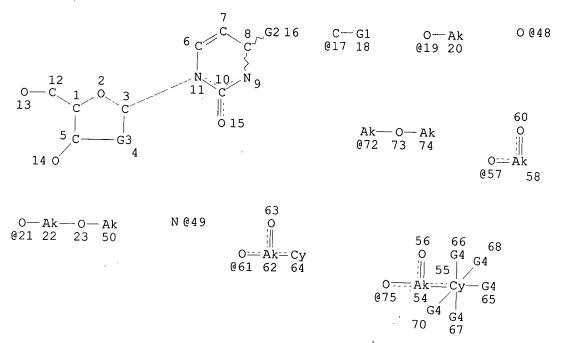
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 4 11
NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE L17 STR



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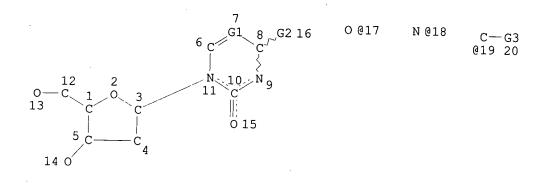
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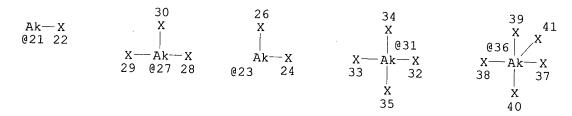
NUMBER OF NODES IS 45

DEFAULT ECLEVEL IS LIMITED

STEREO ATTRIBUTES: NONE

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L19	63849	SEA FILE=REGISTRY ABB=ON PLU	HOL LI
L20	5426	SEA FILE=REGISTRY SUB=L19 CSS	FIII I 1 A
L21	5421	SEA FILE=REGISTRY ABB=ON PLU	EON 130/COM
L22		STR III III ON III	-ON LZU/COM



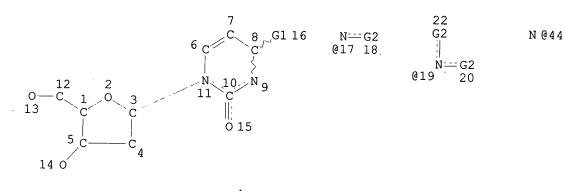


VAR G1=C/19 VAR G2=17/18 VAR G3=X/AK/21/23/27/31/36 NODE ATTRIBUTES: NSPEC IS RC AT 18 CONNECT IS M1 RC AT 4 CONNECT IS M1 RC AT 13 CONNECT IS M1 RC AT 14 CONNECT IS M1 RC AT 18 CONNECT IS M1 RC AT DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 4 11
NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

L23 5421 SEA FILE=REGISTRY SUB=L21 CSS FUL L22 STR



VAR G1=N/17/19/44

VAR G2=AK/CB/23/25/29/33/38

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CONNECT IS M1 RC AT 4
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CONNECT IS M1 RC AT 14
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DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 4 11

NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE

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L40 SCR 2039 OR 2048 OR 2043 OR 2053

L41 885 SEA FILE=REGISTRY SUB=L38 CSS FUL L30 NOT L40

100.0% PROCESSED 885 ITERATIONS

885 ANSWERS

SEARCH TIME: 00.00.01

=> d his

L2

(FILE 'HOME' ENTERED AT 09:04:01 ON 05 JUN 2003) SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:04:25 ON 05 JUN 2003 E US20030032797/PN

L1 1 S E3 SEL RN

FILE 'REGISTRY' ENTERED AT 09:04:44 ON 05 JUN 2003 17 S E1-E17

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 L5
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 L7
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                  SAV TEMP L7 KRI009/A
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                  STR L5
 L9
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 L10
           63750 S L8 CSS FUL SUB=L7
 L11
                 STR L8
 L12
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 L13
            4961 S L11 CSS FUL SUB=L10
 L14
                 STR L11
 L15
            5383 S L14 CSS FUL SUB=L10
 L16
            5378 S L15/COM
                 SAV TEMP L16 KRI009A/A
 L17
                 STR L8
 L18
           63853 S L17 CSS FUL SUB=L7
 L19
           63849 S L18/COM
 L20
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 L21
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L22
                 STR L17
L23
            5421 S L22 CSS FUL SUB=L21
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                 STR L22
L25
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L26
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L27
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L28
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L29
            2036 S L24 NOT L27 CSS FUL SUB=L23
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L30
                 STR L24
L31
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L32
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L33
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L34
               4 S L2 AND L32
L35
               9 S L2 AND L23
               1 S L35 NOT L33, L34
L36
L37
              48 S L30 CSS SAM SUB=L23
L38
            1050 S L30 CSS FUL SUB=L23
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L39
             297 S L38 NOT L32
L40
                 SCR 2039 OR 2048 OR 2043 OR 2053
L41
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L42
              9 S L2 AND L29, L41
            165 S L38 NOT L41
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          11983 S L41
L45
L46
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L47
            482 S L41/P AND L46
L48
            299 S L29 (L) (RCT OR RGT OR RACT)/RL AND L47
L49
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L50 .
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L51
             20 S L48 AND AMINAT?
L52
             39 S L49-L51
L53
             36 S L52 AND (PD<=20010413 OR PRD<=20010413 OR AD<=20010413)
                E MORIZANE K/AU
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L55
               6 S E9
L56
                 E KOUNO T/AU
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L57
L58
               8 S E30
                 E KOMATSU H/AU
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L59
L60
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L61
L62
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          36569 S E3,E4
L63
L64
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L66
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L67
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L71
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L75
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FILE 'REGISTRY' ENTERED AT 11:13:35 ON 05 JUN 2003

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 11:14:03 ON 05 JUN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 5 Jun 2003 VOL 138 ISS 23 FILE LAST UPDATED: 4 Jun 2003 (20030604/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### => d 174 all hitstr tot

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L74 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS
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AN 2003:299012 HCAPLUS

DN 138:304469

TI Method for preparation of cytidine nucleoside derivative

IN Tsuchiya, Katsutoshi; Komatsu, Hironori

PA Mitsui Chemicals Inc., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

IC ICM C07H019-073

ICS A61P031-12; A61P035-00; A61K031-7072

CC 33-9 (Carbohydrates)

Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI OS GI	JP 2003113197 JP 2001-310880 CASREACT 138:304	A2 469	20030418 20011009	JP 2001-310880	20011009

AΒ An efficient process for prepn. of cytidine deriv. is provided which resolves faults in prior art, e.g. a process by prepn. of intermediate 4-(1,2,4-triazol-1-yl)pyrimidin-2-(1H)-one deriv. using toxic phosphorus oxychloride and expensive 2,4,6-triisopropylbenzenesulfonyl chloride followed by amination. Cytidine nucleoside derivs. [I; X = (un) substituted C1-4 alkyl, C2-4 alkenyl, C1-4 haloalkyl; R1, R2 = H, (un) substituted C1-6 alkyl, C5-8 cycloalkyl, (un) substituted benzyl, C1-10 aliph. acyl, (un) substituted arom. acyl, C1-10 aliph. sulfonyl, (un) substituted arom. sulfonyl, (un) substituted silyl; R3 = H, halo, C1-4 alkyl, cyano, alkenyl, alkynyl, (un) substituted OH; R8, R9 = H, (un) substituted C1-6 alkyl, C5-8 cycloalkyl, C2-5 alkenyl; or NR8R9 = pyrrolidino, piperidino, azepan-1-yl, 4-oxopiperidino] are prepd. by reaction of uridine derivs. (II; X, R1-R3 = same as above) with a dehydrating agent and a pyrrolidine deriv. [III; R4 = C1-3 alkyl; R5-R7 =H, each (un)substituted C1-4 alkyl or OH; or R5 and R6 together represent oxo] in the presence of a base followed by amination with NH3 or primary or secondary amine of formula HNR8R9 (R8, R9 = same as above). The intermediates are presumably cytidine quaternary ammonium salts (IV; R1 -R7, X = same as above) which undergo amination with NH3 or primary or secondary amines. Cytidine derivs. are useful as drugs or agrochems. such as anticancer agents and antiviral agents or intermediates for antisense Thus, 1.25 mL triethylamine and 0.88 mL N-methylpyrrolidine were added to a soln. of 2.0 g 3',5'-di-0-(4-chlorobenzoy1)thymidine in 5 mL 1,3-dimethylimidazolidin-2-one (DMI), cooled to 0.degree., treated dropwise with a soln. of 1.54 g p-toluenesulfonyl chloride in 2 mL DMI,

followed by rinsing the reagent into the reaction mixt. 1 mL DMI, and the reaction mixt. was stirred at .ltoreq.10.degree. doe 3 h, cooled to 0.degree., treated dropwise with 8 mL 28% aq. NH3 at .ltoreq.10.degree., stirred at .ltoreq.3.degree. for 3 h, mixed with 10 mL H2O, and extd. twice with EtOAc (20 mL and 10 mL). The ext. was washed three-times with 10 mL H2O, concd., stirred with 20 mL MeOH for 2 h under ice-cooling, and filtered to give, after drying the filtered solid at 40.degree. under reduced pressure 1.78 g 3',5'-di-O-(4-chlorobenzoyl)-5-methyldeoxycytidine (78% yield).

ST cytidine nucleoside prepn intermediate antisense DNA; chlorobenzoylmethyldeoxycytidine prepn antiviral anticancer; uridine condensation pyrrolidine; amination ammonolysis cytidine quaternary ammonium salt

IT Acid halides

RL: RGT (Reagent); RACT (Reactant or reagent)
(acid chlorides, dehydrating agents; prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

IT Dehydration reaction (agents: prepr. of co

(agents; prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

IT Anhydrides

RL: RGT (Reagent); RACT (Reactant or reagent)
(dehydrating agents; prepn. of cytidine nucleoside deriv. by reaction
of uridine deriv. with pyrrolidine deriv. and dehydrating agent
followed by ammonolysis or amination)

IT Antitumor agents

Antiviral agents

(prepn. of cytidine nucleoside deriv. as anticancer or antiviral agent or intermediate for antisense DNA)

IT Antisense DNA

RL: PNU (Preparation, unclassified); PREP (Preparation) (prepn. of cytidine nucleoside deriv. as anticancer or antiviral agent or intermediate for antisense DNA)

IT Amination

Ammonolysis

(prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

IT Deoxyribonucleosides

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

IT Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

IT Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(secondary; prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

IT 98-59-9, p-Toluenesulfonyl chloride

RL: RGT (Reagent); RACT (Reactant or reagent)
(dehydrating agents; prepn. of cytidine nucleoside deriv. by reaction
of uridine deriv. with pyrrolidine deriv. and dehydrating agent
followed by ammonolysis or amination)

IT 110-89-4, Piperidine, reactions 111-49-9, Azepane 120-94-5, N-Methylpyrrolidine 123-75-1, Pyrrolidine, reactions 4449-32-5 7664-41-7, Ammonia, reactions 41661-47-6, 4-Oxopiperidine

#### RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

#### ΙT 367511-34-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

#### IΤ 4449-32-5

#### RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

RN

4449-32-5 HCAPLUS
Thymidine, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

#### IT 367511-34-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of cytidine nucleoside deriv. by reaction of uridine deriv. with pyrrolidine deriv. and dehydrating agent followed by ammonolysis or amination)

RN 367511-34-0 HCAPLUS

Cytidine, 2'-deoxy-5-methyl-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX CN NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \text{H}_2\text{N} \\ & \\ \text{N} \\ & \\ \text{N} \\ & \\ \text{N} \\ & \\ \text{N} \\ & \\ \text{O} \\ & \\ \text{Cl} \\ \end{array}$$

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ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS
L74
     2001:780929 HCAPLUS
ΑN
     135:318660
DN
     Process for the preparation of cytidine derivatives from uridine
ΤI
     derivatives
     Morizane, Kunihiko; Tanikawa, Hiroharu; Kouno,
ΙN
     Toshiyuki; Komatsu, Hironori; Fukazawa, Nobuyuki
     Mitsui Chemicals, Inc., Japan
PΑ
     PCT Int. Appl., 28 pp.
SO
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     Patent
LA
     Japanese
     ICM C07H019-067
IC
     ICS C07H019-073
     33-9 (Carbohydrates)
     Section cross-reference(s): 1
FAN.CNT 1
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                                                             DATE
     PATENT NO.
                      KIND DATE
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     WO 2001079248
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     EP 1186612
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     CASREACT 135:318660; MARPAT 135:318660
OS
GΙ
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Cytidine derivs. (I; X = H, halo, C1-4 alkyl, C1-4 haloalkyl, C2-4 alkenyl; R1, R2 = H, hydroxy-protecting group; R3 = H, halo, H0, C1-4 alkyl, cyano, alkenyl, alkynyl, C1-4 alkoxy, HO substituted by a hydros-protecting group; R4 , R5 = H, C1-4 alkyl, C5-8 cycloalkyl, C1-4 haloalkyl, C2-4 alkenyl; or R4 and R5 are liked together to form a ring) are prepd. by condensation of uridine derivs. (II; X, R1, R2, R3 = same as above) with a tertiary amine and a dehydrating agent and then amination of the intermediate quaternary ammonium salt with NH3 or primary or secondary amine of formula HDR4R5 (R4, R5 = same as above). An efficient synthesis of cytidine derivs. is attained by using a tertiary amine to thereby overcome the disadvantages of the prior art which uses 1,2,4-triazole and requires long reaction time and extn. step. This process shortens reaction time and simplifies procedures and is suitable for large scale prodn. of cytidine derivs. which are useful as anticancer agents and antiviral agents (no data). Thus, 0.23 mL 1-methylpiperidine and 0.45 mL Et3N were added to a soln. of 750 mg 3',5'-O-bis(tert-butyldimethylsilyl)-2'-O-methyluridine in 10 mL MeCN, cooled, treated dropwise with a soln. of 614 mg p-toluenesulfonyl chloride in 5 mL MeCN under ice-cooling, and stirred for 1 h to give an soln. of an intermediate (III). To the latter reaction soln. was added dropwise 3.5 mL 28% aq. NH3 and stirred for 2 h to give 73% 3',5'-0-bis(tertbutyldimethylsilyl) -2'-O-methylcytidine.

ST cytidine deriv prepn antiviral anticancer; amination cytidine quaternary ammonium salt; tertiary amine condensation uridine

IT Amination

(cytidine derivs. by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines

IT Antitumor agents
Antiviral agents

(prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary **amine** with uridine derivs. and **amination** of intermediate quaternary ammonium salt with primary **amines** or secondary **amines**)

IT Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (primary; prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines)

IT Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (secondary; prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines) ΙT 65-71-4, Thymine 121-44-8, Triethylamine, reactions 280-57-9, 1,4-Diazabicyclo[2.2.2]octane 626-67-5, 1-Methylpiperidine 1122-58-3, 4-Dimethylaminopyridine 2140-76-3, 2'-O-Methyluridine 3601-90-9, 3,5-0-Bis(4-chlorobenzoyl)-2-deoxy-D-ribofuranosyl chloride 7664-41-7, Ammonia, reactions 18162-48-6, tert-Butyldimethylsilyl chloride 367511-26-0, 3',5'-O-Bis(4-chlorobenzoy1)-2'-Omethyluridine RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines) 4449-32-5P, 3,5-0-Bis(4-chlorobenzoyl)thymidine ΙT 367511-34-0P 367511-37-3P, 3',5'-O-Bis(tertbutyldimethylsilyl)-2'-O-methyluridine 367511-40-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines) TΤ 5241-10-1P 367511-29-3P 367511-42-0P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines) RE.CNT THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) American Chemical Society; Database CAPLUS on STN (2) American Chemical Society; Database CAPLUS on STN (3) American Chemical Society; Database CAPLUS on STN (4) Mitsui Chemicals Ltd; JP 2000327693 A 2000 HCAPLUS (5) Tokyo Yakka University; JP 06329560 A 1994 HCAPLUS (6) Yamasa Corporation; JP 01143892 A 1989 HCAPLUS 2140-76-3, 2'-O-Methyluridine 367511-26-0, 3',5'-O-Bis(4-chlorobenzoyl)-2'-O-methyluridine RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines)

Uridine, 2'-O-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

2140-76-3 HCAPLUS

RN 367511-26-0 HCAPLUS

Uridine, 2'-O-methyl-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

4449-32-5P, 3,5-0-Bis(4-chlorobenzoyl)thymidine IT367511-34-0P 367511-37-3P, 3',5'-O-Bis(tertbutyldimethylsilyl)-2'-O-methyluridine 367511-40-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of cytidine derivs. as anticancer and antiviral agents by condensation of tertiary amine with uridine derivs. and amination of intermediate quaternary ammonium salt with primary amines or secondary amines)

RN

4449-32-5 HCAPLUS
Thymidine, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

367511-34-0 HCAPLUS RN

Cytidine, 2'-deoxy-5-methyl-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX CN NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \text{H}_2\text{N} \\ & \\ \text{N} \\ & \\ \text{N} \\ & \\ \text{N} \\ & \\ \text{N} \\ & \\ \text{O} \\ & \\ \text{C1} \\ \end{array}$$

RN 367511-37-3 HCAPLUS
CN Uridine, 3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-2'-O-methyl- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 367511-40-8 HCAPLUS
CN Piperidinium, 1-[1-[3,5-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-2-O-methyl-.beta.-D-ribofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

● c1-

IT 5241-10-1P 367511-29-3P 367511-42-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cytidine derivs. as anticancer and antiviral agents by
condensation of tertiary amine with uridine derivs. and
amination of intermediate quaternary ammonium salt with primary
amines or secondary amines)

RN 5241-10-1 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 367511-29-3 HCAPLUS CN Cytidine, 2'-O-methyl-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME)

RN 367511-42-0 HCAPLUS

CN Cytidine, 3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-2'-O-methyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L74 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2001:675221 HCAPLUS

DN 136:6266

TI Large-scale manufacturing of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymatic process

AU Komatsu, Hironori; Awano, Hirokazu; Tanikawa, Hiroharu; Itou, Kiyoshi; Ikeda, Ichirou

CS Chemical Synthesis Laboratory, **Mitsui** Chemicals Inc., Mobara, 297-0017, Japan

SO Nucleosides, Nucleotides & Nucleic Acids (2001), 20(4-7), 1291-1293 CODEN: NNNAFY; ISSN: 1525-7770

PB Marcel Dekker, Inc.

DT Journal

LA English

CC 33-9 (Carbohydrates)
Section cross-reference(s): 7, 9

AB A chem. synthesis of 2-deoxyribose-1-phosphate and its enzymic conversion into purine 2'-deoxynucleosides (dNus) are shown. Besides the chemo-enzymic process for purine dNus, a modified process for practical dC prepn. is also established. Consequently, a series of practical manufg. processes of all four dNus have been realized via novel strategies.

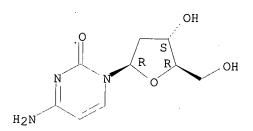
ST deoxynucleoside manufg chemoenzymic coupling nucleobase deoxyribosephosphate

IT Nucleosides, preparation

RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); SPN

(Synthetic preparation); BIOL (Biological study); PREP (Preparation) (deoxynucleosides; large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) IT Coupling reaction (large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) ΙT 958-09-8P, 2'-Deoxyadenosine 961-07-9P, 2'-Deoxyguanosine 3992-42-5P, 2'-Deoxycytidine hydrochloride RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) TΤ 9030-21-1, Purine nucleoside phosphorylase RL: CAT (Catalyst use); USES (Uses) (large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) IT 73-24-5, Adenine, reactions 73-40-5, Guanine 626-67-5. N-Methylpiperidine 10457-14-4, Bis(trimethylsilyl)Uracil 21740-23-8 RL: RCT (Reactant); RACT (Reactant or reagent) (large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) IΤ 5173-91-1P 17039-17-7P **127970-42-7P** RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) RE.CNT THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Friedkin, M; J Biol Chem 1950, V184, P449 HCAPLUS (2) Friedkin, M; J Biol Chem 1950, V184, P461 (3) Kawakami, H; Chem Lett 1989, P235 HCAPLUS (4) Reese, C; Tetrahedron Lett 1980, V21, P2265 HCAPLUS 3992-42-5P, 2'-Deoxycytidine hydrochloride RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (large-scale manufg. of all four 2'-deoxynucleosides via novel strategies including a chemo-enzymic process) RN 3992-42-5 HCAPLUS Cytidine, 2'-deoxy-, monohydrochloride (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry. Rotation (+).



#### HCl

IT 5173-91-1P 127970-42-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (large-scale manufg. of all four 2'-deoxynucleosides via novel
 strategies including a chemo-enzymic process)
RN 5173-91-1 HCAPLUS

Uridine, 2'-deoxy-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME) Absolute stereochemistry.

127970-42-7 HCAPLUS RN Cytidine, 2'-deoxy-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS L74

1990:497957 HCAPLUS ΑN

113:97957 DN

Transformation of uridine derivatives into cytidines via selective TI

ΑU

Krug, A.; Schmidt, S.; Lekhschas, J.; Lemke, K.; Cech, D. Sekt. Chem., Humboldt-Univ. Berlin, Berlin, DDR-1040, Ger. Dem. Rep. CS

Journal fuer Praktische Chemie (Leipzig) (1989), 331(5), 835-42 SO CODEN: JPCEAO; ISSN: 0021-8383

Journal DT

German LA

33-9 (Carbohydrates) CC

CASREACT 113:97957 OS

GI

IT

62420-37-5

288-94-8, 1H-Tetrazole

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with isopropylideneuridine)

RL: RCT (Reactant); RACT (Reactant or reagent)

5-Fluorocytidines I [R = Ac, P(0)(OH)2] were prepd. via amination AΒ of uridine II. 5-Substituted 4-tetrazolopyrimidinones III are key intermediates in the procedure. The method is extended to other fluorinated starting materials, e.g. fluorinated uridine dinucleotide or 2'-deoxy-2'-fluorouridine. The fluoroinated starting materials were prepd. by fluorination with F. ST fluorocytidine; cytidine fluoro; amination fluorouridine; uridine fluoro amination ΙT Amination (regioselective, of fluorouridines) 58-97-9, 5'-Uridylic acid, reactions **58-96-8**, Uridine IT RL: RCT (Reactant); RACT (Reactant or reagent) (fluorination of) ΙT 128963-07-5P 128963-08-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and aminolysis of) TΤ 128963-10-0P 128985-05-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and deacetylation of) TΤ 128963-05**-**3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and fluorination of) 128963-06-4P TΨ 55474-11-8P 67550-04-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and regioselective amination of) IΤ 31535-27-0P 128985-06-8P 10212-20-1P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) IT 2341-22-2P, 5-Fluorocytidine RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from fluorouridine) IT 128963-09-7 RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with chlorophenyl phosphorodichloridate and tetrazole) IT RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with chlorophenyl phosphoroditriazolide)

(reaction of, with nucleosides and chlorophenyl phosphorodichloridate)

IT **58-96-8**, Uridine

RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination of)

RN 58-96-8 HCAPLUS

CN Uridine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 128963-07-5P 128963-08-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and aminolysis of)

RN 128963-07-5 HCAPLUS

CN 2(1H)-Pyrimidinone, 5-fluoro-4-(1H-tetrazol-1-yl)-1-(2,3,5-tri-0-acetyl-beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 128963-08-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-(3,5-di-O-benzoyl-2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)-4-(1H-tetrazol-1-yl)- (9CI) (CA INDEX NAME)

#### IT 128963-10-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and deacetylation of)

RN 128963-10-0 HCAPLUS

CN Cytidine, 5-fluoro-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 55474-11-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(prepn. and regioselective amination of)

RN 55474-11-8 HCAPLUS

CN Uridine, 5-fluoro-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 10212-20-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

10212-20-1 HCAPLUS RN

CN Cytidine, 2'-deoxy-2'-fluoro- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 2341-22-2P, 5-Fluorocytidine

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, from fluorouridine)

RN

2341-22-2 HCAPLUS Cytidine, 5-fluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

ΙT 128963-09-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with chlorophenyl phosphorodichloridate and tetrazole)

128963-09-7 HCAPLUS RN

Uridine, 2'-deoxy-2'-fluoro-, 3',5'-dibenzoate (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

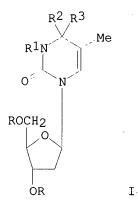
L74 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ΑN 1982:104663 HCAPLUS

DN 96:104663

TI Chemical conversion of thymidine into 5-methyl-2'-deoxycytidine

ΑU Sung, Wing L. CS Div. Biol. Sci., Natl. Res. Counc. Canada, Ottawa, CA, K1A OR6, USA
SO Journal of the Chemical Society, Chemical Communications (1981),
(20), 1089
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
CC 33-9 (Carbohydrates)
Section cross-reference(s): 28
GI



Treating thymidine derivs. I (R = SiMe2CMe3, COMe, R1 = H, R2R3 = O) with 3.0 mol equiv 1,2,4-triazole and 1.5 mol equiv 4-ClC6H4OPOCl2 in pyridine at room temp. 3 days gave 72-73% triazolylpyrimidinones I (R1R2 = bond, R3 = 1,2,4-triazol-1-yl) (II). Treating II with aq. NH3 in dioxane at room temp. 1 h gave 85-89% deoxycytidines I (R = SiMe2CMe3, OH, R1R2 = bond, R3 = NH2).

ST methyldeoxycytidine; deoxycytidine methyl; cytidine deoxy methyl;

thymidine condensation triazole amination IT Condensation reaction

(of thymidine derivs. with triazole, in prepn. of deoxycytidine derivs.)

IT Amination

(of triazolyl nucleosides, methyldeoxycytidines by)

IT Nucleosides, preparation

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of methyldeoxycytidine, from diacetylthymidine via triazolylpyrimidinone nucleoside)

IT 772-79-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation reaction of thymidine derivs. with triazole in presence
 of)

IT 288-88-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation reaction of, with thymidine derivs., in prepn. of
 methyldeoxycytidine derivs.)

IT 6979-97-1 40733-26-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation reaction of, with triazole, in methyldeoxycytidine
 prepn.)

IT 80991-40-8P 80991-41-9P

IT 80991-42-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

IT 838-07-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, from diacetylthymidine via triazolylpyrimidone nucleoside)

IT 6979-97-1 40733-26-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation reaction of, with triazole, in methyldeoxycytidine

prepn.)

RN 6979-97-1 HCAPLUS

CN Thymidine, 3',5'-diacetate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 40733-26-4 HCAPLUS

CN Thymidine, 3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 80991-40-8P 80991-41-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and amination of)

RN 80991-40-8 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-[2-deoxy-3,5-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-5-methyl-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

RN 80991-41-9 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-(3,5-di-O-acetyl-2-deoxy-.beta.-D-erythro-pentofuranosyl)-5-methyl-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 80991-42-0P

RN 80991-42-0 HCAPLUS

CN Cytidine, 2'-deoxy-3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-5-methyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 838-07-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from diacetylthymidine via triazolylpyrimidone nucleoside)

838-07-3 HCAPLUS RN

Cytidine, 2'-deoxy-5-methyl- (6CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS L74

1981:551115 HCAPLUS ΑN

95:151115 DN

ΤI 5-Fluorocytidine

Mitsui Toatsu Chemicals, Inc., Japan PA

Jpn. Kokai Tokkyo Koho, 3 pp. SO

CODEN: JKXXAF

DT Patent

Japanese LA

IC C07H019-06

33-7 (Carbohydrates)

GI

FAN.	CNT 1					
	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
ΡI	JP 56059794	A2	19810523		JP 1979-135939	19791023 <
	JP 62023757	B4	19870525			
DDAT	TD 1979-135939		19791023	<		

The title compd. (I, R = H, R1 = NH2) was prepd. by chlorination of the acylfluorouridine II (R = acyl) followed by **amination** of I (R = acyl) followed by **amination** of I (R = acyl). AΒ acyl, R1 = C1) and subsequent deacylation. Thus, 1.94 g II (R = Ac) in DMF was refluxed with SOC12, the resulting oil treated with NH3-EtOH for 3.5 h, and the product hydrolyzed to give 1.0 g I (R = H, R1 = NH2).

fluorocytidine; cytidine fluoro ST

IT 55474-11-8

RL: RCT (Reactant); RACT (Reactant or reagent) (chlorination of)

ΙT 79343-28-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and amination of)

IT 2341-22-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

IT 55474-11-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(chlorination of)

RN 55474-11-8 HCAPLUS

CN Uridine, 5-fluoro-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 2341-22-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 2341-22-2 HCAPLUS

CN Cytidine, 5-fluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L74 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 1980:198686 HCAPLUS

DN 92:198686

TI 2'-Deoxy-5-methylcytidine. Amination of thymidine

AU Vorbrueggen, Helmut; Krolikiewicz, Konrad

CS Schering A.-G., Berlin, 1000/65, Fed. Rep. Ger.

Nucl. Acid Chem. (1978), Volume 1, 227-9. Editor(s): Townsend, Leroy B.; Tipson, R. Stuart. Publisher: Wiley, New York, N. Y. CODEN: 42TBAU

DT Conference

LA English

CC 33-7 (Carbohydrates)

GI

AB A mixt. of thymidine, hexamethyldisilazane, HCONH2, and (NH4)2SO4 was autoclaved 72 h at 130-5.degree., and the product was refluxed with MeOH to give after silica column chromatog. 75% deoxymethylcytidine I.

ST deoxymethylcytidine; cytidine deoxy methyl; amination thymidine

IT Amination

(of thymidine, deoxymethycytidine from)

IT **50-89-5**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(amination of, deoxymethylcytidine from)

IT 838-07-3P 5241-10-1P

Ι

IT **50-89-5**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(amination of, deoxymethylcytidine from)

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 838-07-3P 5241-10-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 838-07-3 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

RN 5241-10-1 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

```
ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS
L74
ΑN
     1979:23542 HCAPLUS
DN
     90:23542
     2'-Deoxy-5-methylcytidine: Amination of thymidine
TI
     Vorbrueggen, Helmut; Krolikiewicz, Konrad
AU
     Schering A.-G., Berlin, Fed. Rep. Ger.
CS
     Nucleic Acid Chem. (1978), Volume 1, 227-9. Editor(s):
SO
     Townsend, Leroy B.; Tipson, R. Stuart. Publisher: Wiley, New York, N. Y.
     CODEN: 39GCA6
DT
     Conference
LA
     English
     33-7 (Carbohydrates)
CC
     Autoclaving thymidine, (Me3Si)2NH, HCONH2, and (NH4)2SO4 at 130-5.degree.
AB
     for 72 h gave 75% 2'-deoxy-5-methylcytidine, which was converted to the
     hydrochloride and recrystd. from EtOH.
     deoxymethylcytidine; cytidine deoxy methyl; amination thymidine
ST
ΙT
     Amination
        (of thymidine, 2'-deoxy-5-methylcytidine from)
ΙT
     50-89-5, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (amination of, 2'-deoxy-5-methylcytidine from)
IT
     838-07-3P 68696-19-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
ΙT
     50-89-5, reactions
```

RL: RCT (Reactant); RACT (Reactant or reagent)

(amination of, 2'-deoxy-5-methylcytidine from)

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 838-07-3P 68696-19-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 838-07-3 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 68696-19-5 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl-, hydrochloride (6CI, 9CI) (CA INDEX NAME)

### => d all hitstr tot

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ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2003 ACS
ΑN
     2002:314958 HCAPLUS
DN
     Preparation of modified nucleosides for treatment of viral infections and
ΤI
      abnormal cellular proliferation
     Stuyver, Lieven; Watanabe, Kyoichi A.
IN
      Pharmasset Limited, USA
PΑ
      PCT Int. Appl., 230 pp.
SO
      CODEN: PIXXD2
DT
      Patent
LA
      English
      ICM C07H019-00
IC
CC
      33-9 (Carbohydrates)
      Section cross-reference(s): 1, 7, 10, 63
FAN.CNT 2
                                                  APPLICATION NO.
                                                                       DATE
                          KIND
                                 DATE
      PATENT NO.
      _____
                                 20020425
                                                  WO 2001-US46113
                                                                       20011018 <--
    . WO 2002032920
                          A2
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
               CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
               LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
               RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU,
                                                                   TZ, UA, UG, US, UZ,
                                                                   TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
               BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                                 20020429
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      US 2003087873
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                                 20030508
                                 20001018
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                           Ρ
PRAI US 2000-241488P
                           Р
                                 20010406
                                             <--
      US 2001-282156P
                                 20011018
      WO 2001-US46113
                           W
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Ι

GΙ

Modified nucleosides, e.g. I, wherein D is hydrogen, alkyl, acyl, monophosphate, diphosphate, triphosphate, monophosphate ester, diphosphate ester, triphosphate ester, phospholipid or amino acid; X is H, halogen, NH2, substituted amine, oxime, OH, alkoxy, SH, thioalkyl; Y is O, S, Se; R and R1 are independently H, alkyl, alkenyl, alkynyl, aryl, alkylaryl, halogen, NH2, substituted amine, oxime, hydrazine, OH, alkoxy, SH, thioalkyl, NO2, NO, CH2OH, CH2OH, ester, CONH2, amide, CN; R2 and R3 are independently H, halogen, OH, SH, OMe, SMe, NH2, NHMe,

ST

ΙT

IT

IT

ΙT

IT

181785-90-0P

221617-05-6P

181785-91-1P

224317-26-4P

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CH:CH2, CN, CH2NH2, CH2OH, CO2H; were prepd. for treating a Flaviviridae
(including BVDV and HCV), Orthomyxoviridae (including Influenza A and B)
or Paramyxoviridae (including RSV) infection, or conditions related to
abnormal cellular proliferation, in a host, including animals, and esp.
humans. This invention also provides an effective process to quantify the
viral load, and in particular BVDV, HCV or West Nile Virus load, in a
host, using real-time polymerase chain reaction ("TR-PCR"). Addnl., the
invention discloses probe mols. that can fluoresce proportionally to the
amt. of virus present in a sample. Thus, (1'R, 2'S, 3'R, 4'R)-1-[2, 3-1]
dihydroxy-4-(hydroxymethyl)cyclopentan-1-yl]-5-fluorocytosine was prepd.
and tested in vitro as antiviral and antitumor agent.
cytotoxicity nucleoside prepn antiviral antitumor human antiinfluenza;
polymerase chain reaction nucleoside prepn antiviral antitumor human
antiinfluenza; nucleoside prepn antiviral antitumor human antiinfluenza
Orthomyxoviridae Paramyxoviridae Flaviviridae
Antitumor agents
Antiviral agents
Cytotoxicity
Human
PCR (polymerase chain reaction)
West Nile virus
   (prepn. of modified nucleosides for treatment of viral infections and
   abnormal cellular proliferation)
Nucleosides, preparation
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
   (prepn. of modified nucleosides for treatment of viral infections and
   abnormal cellular proliferation)
Bovine diarrhea virus
Flaviviridae
Hepatitis C virus
Influenza A virus
Influenza B virus
Orthomyxoviridae
Paramyxoviridae
   (treatment; prepn. of modified nucleosides for treatment of viral
   infections and abnormal cellular proliferation)
   (viral, treatment; prepn. of modified nucleosides for treatment of
   viral infections and abnormal cellular proliferation)
           73-03-0P 131-06-6P 147-94-4P
50-91-9P
316-46-1P
            727-79-7P
                        957-77-7P
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5399-87-1P
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193754-19-7P

241806-22-4P

196085-98-0P

241806-28-0P

210474-57-0P

259261-22-8P

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     RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN
     (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
     PREP (Preparation); USES (Uses)
        (prepn. of modified nucleosides for treatment of viral infections and
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                                                   415705-82-7P
ΙT
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     415705-84-9P
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                  3258-02-4P 3803-28-9P
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     25383-84-0P
                                                52482-84-5P
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     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
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        (prepn. of modified nucleosides for treatment of viral infections and
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ΙT
     51-21-8, 5-Fluorouracil
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               65-71-4, Thymine
                                   87-42-3, 6-Chloropurine
                                                            1005-56-7, Phenyl
                           3106-03-4, 5-Nitrouridine 3768-18-1
                                                                    5432-33-7
     chlorothionoformate
                                                              10526-27-9
     6553-96-4, 2,4,6-Triisopropylbenzenesulfonyl chloride
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ΙT

20031-21-4 42927-46-8 128114-98-7 223596-25-6 415704-42-6 RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of modified nucleosides for treatment of viral infections and abnormal cellular proliferation) ΙT 417196-38-4 417196-39-5 417196-40-8 417196-37-3 417196-41-9 417196-42-0 RL: PRP (Properties) (unclaimed sequence; prepn. of modified nucleosides for treatment of viral infections and abnormal cellular proliferation) 50-91-9P 131-06-6P 147-94-4P 316-46-1P ΙT 2341-22-2P 3066-86-2P 4298-10-6P 10212-19-8P 17676-66-3P 27921-78-4P 32791-81-4P 57729-40-5P 58461-30-6P 58461-34-0P 77180-78-0P 77210-26-5P 77210-27-6P 83966-93-2P 374107-80-9P 415704-56-2P 415704-57-3P 415704-62-0P 415704-64-2P 415704-70-0P 415704-81-3P 415704-82-4P 415704-89-1P 415704-90-4P 415704-91-5P RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of modified nucleosides for treatment of viral infections and abnormal cellular proliferation) RN 50-91-9 HCAPLUS Uridine, 2'-deoxy-5-fluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN 131-06-6 HCAPLUS CN 2,4(1H,3H)-Pyrimidinedione, 1-.beta.-D-arabinofuranosyl-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 147-94-4 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 316-46-1 HCAPLUS CN Uridine, 5-fluoro- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 2341-22-2 HCAPLUS CN Cytidine, 5-fluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 3066-86-2 HCAPLUS CN Cytidine, 5-bromo- (7CI, 8CI, 9CI) (CA INDEX NAME)

RN 4298-10-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 10212-19-8 HCAPLUS

CN Cytidine, 2'-chloro-2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 17676-66-3 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl-5-bromo- (9CI) (CA INDEX NAME)

RN 27921-78-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-L-arabinofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 32791-81-4 HCAPLUS

CN Cytidine, 2'-bromo-2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 57729-40-5 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-(2,3,5-tri-O-acetyl-.beta.-D-xylofuranosyl)- (9CI) (CA INDEX NAME)

RN 58461-30-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-chloro-2-deoxy-.beta.-D-arabinofuranosyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 58461-34-0 HCAPLUS

CN Cytidine, 2'-chloro-2'-deoxy-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 77180-78-0 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-.beta.-L-erythro-pentofuranosyl)-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 77210-26-5 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-.beta.-L-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 77210-27-6 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-.beta.-L-arabinofuranosyl-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 83966-93-2 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-bromo-2-deoxy-.beta.-D-arabinofuranosyl)-5-iodo- (9CI) (CA INDEX NAME)

RN 374107-80-9 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-L-arabinofuranosyl-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 415704-56-2 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-chloro-2-deoxy-.beta.-L-ribofuranosyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 415704-57-3 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-bromo-2-deoxy-.beta.-L-ribofuranosyl)(9CI) (CA INDEX NAME)

RN 415704-62-0 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-chloro-2-deoxy-.beta.-L-arabinofuranosyl)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 415704-64-2 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-5-fluoro-1-.beta.-L-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 415704-70-0 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-chloro-2-deoxy-.beta.-L-ribofuranosyl)-5-fluoro- (9CI) (CA INDEX NAME)

RN 415704-81-3 HCAPLUS CN 2(1H)-Pyrimidinone, 4-amino-5-bromo-1-.beta.-L-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 415704-82-4 HCAPLUS CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-L-arabinofuranosyl-5-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 415704-89-1 HCAPLUS CN Cytidine, 2'-chloro-2'-deoxy-5-iodo- (9CI) (CA INDEX NAME)

RN 415704-90-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-chloro-2-deoxy-.beta.-L-ribofuranosyl)-5-iodo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 415704-91-5 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-bromo-2-deoxy-.beta.-L-arabinofuranosyl)-5-iodo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# IT 3803-28-9P 14057-25-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of modified nucleosides for treatment of viral infections and abnormal cellular proliferation)

RN 3803-28-9 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-.beta.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

RN 14057-25-1 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-methyl-1-(2,3,5-tri-O-acetyl-.beta.-D-xylofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT **58-96-8**, Uridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of modified nucleosides for treatment of viral infections and abnormal cellular proliferation)

RN 58-96-8 HCAPLUS

CN Uridine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 2002:180164 HCAPLUS

DN 137:47389

TI Synthesis of N4-alkyl-5-methyl-2'-deoxycytidine

AU Yu, Jianxin; Zhang, Wannian; Zhu, Ju; Lu, Jiaguo; Li, Ke

CS Department of Pharmacy, Second Military Medical University, Shanghai, 200433, Peop. Rep. China

SO Zhongguo Yiyao Gongye Zazhi (2001), 32(12), 547-549 CODEN: ZYGZEA; ISSN: 1001-8255

PB Zhongguo Yiyao Gongye Zazhi Bianjibu

DT Journal

LA Chinese

CC 33-9 (Carbohydrates)

OS CASREACT 137:47389

```
A series of new N4-alkyl-5-methyl-2'-deoxytidines were synthesized by
 AB
      displacement of triazole group at C4 of 1-(3',5'- O-dibenzoyl-.beta.-D-
      ribofuranosyl)-4-(1,2,4-triazol-1-yl)-5-methyl-pyrimidin-2(1H)-one, which
      was obtained by condensation of 3',5'-O-dibenzoylthymidine with
      1,2,4-triazole in the presence of POC13.
 ST
      alkyl methyldeoxycytidine prepn substitution reaction
 ΙT
      Heterocyclic compounds
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (nitrogen; synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
 IT
      Substitution reaction
         (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
IT
     Nucleosides, preparation
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
IT
     10025-87-3, Phosphoric trichloride
     RL: CAT (Catalyst use); USES (Uses)
         (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
IT
     75-31-0, Isopropyl amine, reactions 98-88-4, Benzoyl chloride
     104-94-9, 4-Methoxyphenyl amine
                                       107-11-9, Allyl amine
     25406-45-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
TΤ
     50-89-5P, Thymidine, preparation 78138-02-0P 438588-33-1P 4385
                                         288-88-0P, 1H-1,2,4-Triazole
                                   438588-41-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (synthesis of N4-alkyl-5-methyl-2-deoxycytidine)
ΙT
     25406-43-3P 25406-44-4P
                                104579-02-4P
     438588-38-6P 438588-39-7P 438588-40-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
ΙT
     25406-45-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)
RN
     25406-45-5 HCAPLUS
     Cytidine, 2'-deoxy-N,N,5-trimethyl- (8CI, 9CI) (CA INDEX NAME)
CN
```

Absolute stereochemistry.

IT 25406-43-3P 25406-44-4P 438588-38-6P 438588-39-7P 438588-40-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of N4-alkyl-5-methyl-2'-deoxycytidine)

RN 25406-43-3 HCAPLUS

CN Cytidine, 2'-deoxy-N-ethyl-5-methyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 25406-44-4 HCAPLUS CN Cytidine, 2'-deoxy-N,5-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 438588-38-6 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 438588-39-7 HCAPLUS CN Cytidine, 2'-deoxy-5-methyl-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 438588-40-0 HCAPLUS CN Cytidine, 2'-deoxy-5-methyl-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:251183 HCAPLUS

DN 128:321868

TI Improved coupling activators for oligonucleotide synthesis

IN Vargeese, Chandra; Pieken, Wolfgang; Carter, Jeffrey D.; Yegge, John

PA Nexstar Pharmaceuticals, Inc., USA; Vargeese, Chandra; Pieken, Wolfgang;

Carter, Jeffrey D.; Yegge, John SO PCT Int. Appl., 50 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07H021-00

```
ICS C07H021-04; C07H001-00
CC
     33-10 (Carbohydrates)
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                          APPLICATION NO. DATE
                      ----
PΙ
     WO 9816540
                      A1
                            19980423
                                           WO 1997-US15744 19971008 <--
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG,
             US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
     AU 9748001
                      A1 19980511
                                           AU 1997-48001
                                                            19971008 <--
PRAI US 1996-730556
                            19961015
                                      <---
     US 1997-937867
                            19970925
                                     <--
     WO 1997-US15744
                            19971008 <--
     A method for coupling phosphoramidite monomers with nucleophiles, for
     example, the 5'-hydroxyl group on the growing oligonucleotide chain, using
     a coupling activator that is less acidic than and at least as nucleophilic
     as tetrazole and that provides comparable or better coupling efficiency
     than tetrazole. The pKa of the coupling activator is between 5.0 and 6.0,
     preferably between 5.0 and 5.5, and, more preferably, between 5.1 and 5.3.
     Suitable coupling activators include 4,5-dicyanoimidazole (DCI),
     4-alkylthioimidazole, 2-alkylthioimidazole, 2-nitroimidazole,
     4-nitroimidazole, 4,5-dihaloimidazole, 4-haloimidazole, 2-haloimidazole
     and 5-alkoxytetrazole. DCI is the most preferred coupling activator.
     Alternatively, a combination of an acidic coupling activator and a
     suitable buffer, such as a tertiary amine, can be employed.
     tertiary amine can be a tertiary amine with three
     alkyl groups or a heterocyclic compd. contg. one or more tertiary
     amines. Preferably the tertiary amine is less
     nucleophilic than DMAP, which is known to cause side reactions at the
     6-position oxygen of guanosines due to its relatively high
     nucleophilicity. N-methylimidazole (NMI) is the preferred tertiary
ST
     oligodeoxyribonucleotide synthesis coupling activator imidazole
ΙT
     Oligodeoxyribonucleotides
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (improved imidazole coupling activators for oligodeoxyribonucleotide
        synthesis)
ΙT
     Coupling reaction
        (improved imidazole coupling activators for oligonucleotide synthesis)
IT
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
        (improved imidazole coupling activators for oligonucleotide synthesis)
IT
     10212-20-1P
                   205454-24-6P
                                  205454-25-7P
                                                 205454-26-8P
     205454-27-9P
                    206887-59-4P
                                   206887-60-7P
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (improved imidazole coupling activators for oligonucleotide synthesis)
ΙT
     1122-28-7P, 1H-Imidazole-4,5-dicarbonitrile
     RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation);
     RACT (Reactant or reagent)
        (improved imidazole coupling activators for oligonucleotide synthesis)
     288-94-8, 1H-Tetrazole 616-47-7, N-Methylimidazole 10212-13-2
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (improved imidazole coupling activators for oligonucleotide synthesis)
RE.CNT
              THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Reddy; US 5574146 A 1996 HCAPLUS
```

#### ΙT 10212-20-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(improved imidazole coupling activators for oligonucleotide synthesis)

RN10212-20-1 HCAPLUS

Cytidine, 2'-deoxy-2'-fluoro- (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

### ΙT 10212-13-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(improved imidazole coupling activators for oligonucleotide synthesis)

10212-13-2 HCAPLUS RN

Uridine, 2'-deoxy-2'-fluoro-, 3',5'-diacetate (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2003 ACS L75

1997:259665 HCAPLUS AN

DN 126:277718

One-pot synthesis of 4-aminopyrimidine nucleoside from 4-hydroxypyrimidine ΤI nucleoside

IN Mori, Takeya

Yamasa Shoyu Kk, Japan PA

Jpn. Kokai Tokkyo Koho, 3 pp. SO

CODEN: JKXXAF

DTPatent

LA Japanese

ICM C07H019-06 IC

33-9 (Carbohydrates) CC

FAN.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PRAI	JP 09059292 JP 1995-240927 CASREACT 126:277	A2	19970304 19950825 <		19950825 <

OS GΙ

AΒ The title compds. (I; R1 = H, lower alkyl, halo; R2 - R5 = H, OH) are prepd. by protecting hydroxy groups of 4-hydroxypyrimidine nucleosides (II; R1 - R5 = same as above) with trimethylsilyl group and subsequent reaction with phosphorus oxychloride or 4-chlorophenyl phosphorodichloridate and amination with aq. NH3 without isolating the resulting intermediate. The procedures of this process are simpler than those of prior art and the reaction can be carried out under mild conditions in one pot. Thus, 5.1 mL trimethylsilyl chloride was added to a soln. of 2.44 g uridine in 50 mL pyridine, stirred at room temp. for 1 h, followed by adding 2 mL POCl3, and the resulting mixt. was stirred at room temp. for 4 h. To the reaction mixt. was added 5 mL ice-cooled H2O at 0.degree. and after stirring the mixt. for 30 min, 20 mL 25 aq. NH3 was added and stirred at 50.degree. for 2 h to give, after purifn. using ion exchange resin PK216, 83.9% cytidine. Similarly prepd. were 5-methylcytidine and 5-bromocytidine from 5-methyluridine and 5-bromouridine, resp.

aminopyrimidine nucleoside one pot prepn; hydroxypyrimidine nucleoside amination; phosphorus oxychloride condensation hydroxypyrimidine nucleoside; trimethylsilylation hydroxypyrimidine nucleoside

IT Pyrimidine nucleosides

RL: SPN (Synthetic preparation); PREP (Preparation) (One-pot synthesis of aminopyrimidine nucleosides from hydroxypyrimidine nucleosides)

TT 58-96-8, Uridine 75-77-4, Trimethylsilyl chloride, reactions 772-79-2, 4-Chlorophenyl phosphorodichloridate 957-75-5, 5-Bromouridine 1463-10-1, 5-Methyluridine 7664-41-7, Ammonia, reactions 10025-87-3, Phosphorus oxychloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(One-pot synthesis of aminopyrimidine nucleosides from hydroxypyrimidine nucleosides)

IT 65-46-3P, Cytidine 2140-61-6P, 5-Methylcytidine 3066-86-2P, 5-Bromocytidine

RL: SPN (Synthetic preparation); PREP (Preparation) (One-pot synthesis of aminopyrimidine nucleosides from hydroxypyrimidine nucleosides)

IT 58-96-8, Uridine 957-75-5, 5-Bromouridine

**1463-10-1**, 5-Methyluridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(One-pot synthesis of aminopyrimidine nucleosides from hydroxypyrimidine nucleosides)

RN 58-96-8 HCAPLUS

CN Uridine (8CI, 9CI) (CA INDEX NAME)

RN 957-75-5 HCAPLUS CN Uridine, 5-bromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 1463-10-1 HCAPLUS CN Uridine, 5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 65-46-3P, Cytidine 2140-61-6P, 5-Methylcytidine 3066-86-2P, 5-Bromocytidine

RL: SPN (Synthetic preparation); PREP (Preparation) (One-pot synthesis of aminopyrimidine nucleosides from hydroxypyrimidine nucleosides)

RN 65-46-3 HCAPLUS

CN Cytidine (8CI, 9CI) (CA INDEX NAME)

RN 2140-61-6 HCAPLUS

Cytidine, 5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

3066-86-2 HCAPLUS RN

CN Cytidine, 5-bromo- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2003 ACS

ΑN 1995:614105 HCAPLUS

DN 123:314326

Direct synthesis, substitution, and structure of 1-(2'-deoxy-.beta.-D-TΙ  $\verb|erythro-pentofuranosyl|| -4-pentafluorophenylpyrimidin-2H-one||$ 

Wallis, Mark P.; Spiers, Ian D.; Schwalbe, Carl H.; Fraser, William ΑU

Pharmaceutical Sci. Inst., Aston Univ., Birmingham, B4 7ET, UK CS

Tetrahedron Letters (1995), 36(21), 3759-62 SO CODEN: TELEAY; ISSN: 0040-4039

PΒ Elsevier

DTJournal

LA English

CC 33-9 (Carbohydrates)

GΙ

AB Direct methods have been developed to access the title nucleoside I from 2'-deoxyuridine. The C-4 pentafluorophenyl group of I is readily displaced by amine nucleophiles forming N-4 substituted cytosines in good to excellent yields.

amine nucleophilic substitution pentafluorophenylpyrimidinone nucleoside; nucleoside pentafluorophenylpyrimidinone prepn mol structure; deoxypentofuranosyl pentafluorophenylpyrimidinone prepn mol structure

IT Substitution reaction, nucleophilic

Substitution reaction, nucleophilic (synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

IT Nucleosides, preparation

Ι

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

1T 64-04-0, Benzeneethanamine 589-08-2, N-MethylBenzeneethanamine 771-61-9, Pentafluorophenol. 951-78-0, 2'-Deoxyuridine 83392-10-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

IT 109389-24-4P 170114-35-9P 170114-39-3P 170114-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

IT 104105-76-2P 170114-36-0P 170114-37-1P 170114-38-2P

170114-40-6P RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

IT 951-78-0, 2'-Deoxyuridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

RN 951-78-0 HCAPLUS

CN Uridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

109389-24-4P ΙT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

109389-24-4 HCAPLUS RN

2(1H)-Pyrimidinone, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-4-(1H-CN 1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

104105-76-2P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis and substitution and mol. structure of deoxypentofuranosyl pentafluorophenylpyrimidinone)

104105-76-2 HCAPLUS RN

2(1H)-Pyrimidinone, 1-.beta:-D-ribofuranosyl-4-(1H-1,2,4-triazol-1-yl)-CN (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2003 ACS

1995:224840 HCAPLUS AN

122:240302 DN

A new and efficient synthesis of cytidine and adenosine derivatives by ΤI dimethyldioxirane oxidation of thiopyrimidine and thiopurine nucleosides

```
Saladino, Raffaele; Crestini, Claudia; Bernini, Roberta; Frachey,
 AII
      Giuseppe; Mincione, Enrico
      Dipartimento Agrochimico Agrobiologico, Universita degli studi di Viterbo
 CS
      La Tuscia, Viterbo, 01100, Italy
      Journal of the Chemical Society, Perkin Transactions 1: Organic and
 SO
      Bio-Organic Chemistry (1994), (21), 3053-4
      CODEN: JCPRB4; ISSN: 0300-922X
 PΒ
      Royal Society of Chemistry
 DT
      Journal
      English
 LA
      33-9 (Carbohydrates)
 CC
      CASREACT 122:240302
 OS
     Dimethyldioxirane oxidn. of thiopyrimidine and thiopurine nucleosides, in
 AΒ
     the presence of amines in stoichiometric amt., afforded
     selectively and under mild exptl. conditions cytidine and adenosine
      nucleosides.
ST
     thiopurine nucleoside stereoselective oxidn dimethyldioxirane;
     dimethyldioxirane stereoselective oxidn thiopyrimidine nucleoside
ΙT
     Oxidation
     Stereochemistry
         (synthesis of cytidine and adenosine derivs. by dimethyldioxirane
        oxidn. of thiopyrimidine and thiopurine nucleosides)
IT
     Nucleosides, preparation
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (synthesis of cytidine and adenosine derivs. by dimethyldioxirane
        oxidn. of thiopyrimidine and thiopurine nucleosides)
IT
     50-89-5, Thymidine, reactions 58-96-8, Uridine
                3021-21-4
                            153336-41-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of cytidine and adenosine derivs. by dimethyldioxirane
        oxidn. of thiopyrimidine and thiopurine nucleosides)
ΙT
     7387-57-7P
                  20188-74-3P
                                55003-25-3P 56787-28-1P
     65919-98-4P
                   103931-23-3P 111426-20-1P
     115652-25-0P 162210-81-3P
                                162210-82-4P
                                                162210-85-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis of cytidine and adenosine derivs. by dimethyldioxirane
        oxidn. of thiopyrimidine and thiopurine nucleosides)
     58-61-7P, Adenosine, preparation 65-46-3P, Cytidine
ΙT
     838-07-3P 951-77-9P
                           2096-10-8P 10578-79-7P
     162210-83-5P
                    162210-84-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of cytidine and adenosine derivs. by dimethyldioxirane
        oxidn. of thiopyrimidine and thiopurine nucleosides)
ΙT
     50-89-5, Thymidine, reactions 58-96-8, Uridine
     951-78-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of cytidine and adenosine derivs. by dimethyldioxirane
        oxidn. of thiopyrimidine and thiopurine nucleosides)
RN
     50-89-5 HCAPLUS
CN
     Thymidine (8CI, 9CI) (CA INDEX NAME)
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58-96-8 HCAPLUS RN (CA INDEX NAME) Uridine (8CI, 9CI) CN

Absolute stereochemistry.

951-78-0 HCAPLUS RNUridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

56787-28-1P 65919-98-4P 111426-20-1P ΙT

115652-25-0P 162210-81-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of cytidine and adenosine derivs. by dimethyldioxirane oxidn. of thiopyrimidine and thiopurine nucleosides)

56787-28-1 HCAPLUS RN

Cytidine, 2',3',5'-triacetate (7CI, 9CI) (CA INDEX NAME) CN

RN 65919-98-4 HCAPLUS

CN Cytidine, 2'-deoxy-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111426-20-1 HCAPLUS

CN Cytidine, N-methyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 115652-25-0 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 162210-81-3 HCAPLUS

CN Cytidine, N-propyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 65-46-3P, Cytidine 838-07-3P 951-77-9P 10578-79-7P 162210-83-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of cytidine and adenosine derivs. by dimethyldioxirane oxidn. of thiopyrimidine and thiopurine nucleosides)

RN 65-46-3 HCAPLUS

CN Cytidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838-07-3 HCAPLUS CN Cytidine, 2'-deoxy-5-methyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 951-77-9 HCAPLUS CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 10578-79-7 HCAPLUS

CN Cytidine, N-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 162210-83-5 HCAPLUS

CN Cytidine, N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1995:65930 HCAPLUS

DN 122:81860

TI Oxidation of nucleic acid related compounds by the peroxodisulfate ion

AU Itahara, Toshio; Yoshitake, Takashi; Koga, Sunao; Nishino, Akihiro

CS College Lib. Arts, Kagoshima Univ., Kagoshima, 890, Japan

SO Bulletin of the Chemical Society of Japan (1994), 67(8), 2257-64 CODEN: BCSJA8; ISSN: 0009-2673

DT Journal

LA English

CC 33-9 (Carbohydrates)

The treatment of nucleic acid bases, nucleosides, and nucleotides with peroxodisulfate ion in a phosphate buffer soln. at pH 7.0 or water at 70-75 .degree.C was investigated. The reaction of thymine and 5-methylcytosine nucleosides and nucleotides resulted in the oxidn. of the 5-Me groups. The oxidn. products from 1,3-dimethyluracils and the time-course of the reaction of uracils led to two plausible reaction mechanisms for the oxidn. of uracils.

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nucleic acid oxidn peroxodisulfate; nucleobase oxidn peroxodisulfate;
ST
    nucleotide oxidn peroxodisulfate; nucleoside oxidn peroxodisulfate
     Nucleic acid bases
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
ΙT
     Oxidation
        (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)
     Nucleosides, reactions
IT
     Nucleotides, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)
                                     58-61-7, Adenosine, reactions
     50-89-5, Thymidine, reactions
TΤ
     58-96-8, Uridine 65-46-3, Cytidine
                                          66-22-8,
                                             71-30-7
                                                       73-24-5, 1H-Purin-6-
     2,4(1H,3H)-Pyrimidinedione, reactions
                       874-14-6 951-77-9 951-78-0
     amine, reactions
                                                                  61240-13-9
                                                    18531-27-6
                            4401-71-2
                                        7033-39-8
     958-09-8
                3013-92-1
                                               160509-70-6 160509-76-2
                   108321-45-5
                                 160509-67-1
     108320-84-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)
     137017-45-9P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)
     65-71-4P 120-89-8P, Imidazolidinetrione
                                                132-00-3P 838-07-3P
IT
                  1195-08-0P
                                             3106-18-1P
                                                         4425-59-6P
                               2835-45-2P
     1123-95-1P
                                                          5176-82-9P
                               4869-46-9P
                                             5116-24-5P
     4433-40-3P
                  4494-26-2P
                                              15718-50-0P
                                                             20406-86-4P
                                14181-46-5P
     7226-77-9P
                  13509-52-9P
                                                               160509-68-2P
                                                138610-55-6P
                                 107097-10-9P
     20636-41-3P
                   56070-36-1P
                                                                  160509-74-0P
                                                  160509-73-9P
                                   160509-72-8P
                    160509-71-7P
     160509-69-3P
                    160509-77-3P
     160509-75-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)
     50-89-5, Thymidine, reactions 58-96-8, Uridine
IT
     65-46-3, Cytidine 951-77-9 951-78-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)
RN
     50-89-5 HCAPLUS
     Thymidine (8CI, 9CI) (CA INDEX NAME)
CN
```

Absolute stereochemistry.

RN 58-96-8 HCAPLUS CN Uridine (8CI, 9CI) (CA INDEX NAME)

RN 65-46-3 HCAPLUS CN Cytidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 951-77-9 HCAPLUS CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 951-78-0 HCAPLUS CN Uridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

## IT 838-07-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (oxidn. of nucleic acid related compds. by the peroxodisulfate ion)

RN 838-07-3 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1991:7050 HCAPLUS

DN 114:7050

TI Improved procedure for the regiospecific synthesis of 2'-deoxyribonucleosides

AU Baud, M. V.; Chavis, C.; Lucas, M.; Imbach, J. L.

CS Lab. Chim. Bio-Org., Univ. Montpellier II, Montpellier, 34095, Fr.

SO Tetrahedron Letters (1990), 31(31), 4437-40

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

CC 33-9 (Carbohydrates)

OS CASREACT 114:7050

GI

AB 2'-Deoxyribonucleosides are regiospecifically synthesized in high yields by the KI-dibenzo-18-crown-6 phase-transfer catalyzed condensation of unprotected silylated purines and pyrimidines with 2-deoxyribofuranosyl or

```
pyranosyl acetates. Thus, dibenzoyldeoxyfuranosyl acetates I were treated
    with trimethylsilylated adenine in the presence of KI-dibenzo-8-crown-6 in
    MeCN-PhMe to give 95% a mixt. of .alpha.- and .beta.-2'-deoxynucleosides
    II and III (R = Bz). Treatment with NH3-MeOH quant. gave II and III (R =
    deoxyribonucleoside regioselective prepn pyrimidine; nucleoside deoxyribo;
ST
    benzoyldeoxyfuranosyl acetate condensation silylated purine pyrimidine;
    benzoyldeoxypyranosyl acetate condensation silvlated purine pyrimidine
    Regiochemistry
IT
        (of condensation of silylated purines and pyrimidines with
        benzoylfuranosyl or -pyranosyl acetates)
    Condensation reaction
ΙT
        (of silylated purines or pyrimidines with benzoylfuranosyl or
        -pyranosyl acetates, nucleosides from)
     Nucleosides, preparation
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (deoxyribo-, prepn. of, by condensation of silylated purines or
        pyrimidines with benzoylfuranosyl or -pyranosyl acetates)
     65-71-4D, Thymine, silylated 71-30-7D, Cytosine, silylated
TT
                                   73-40-5D, Guanine, silylated
     1H-Purin-6-amine, silylated
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with benzoylfuranosyl or -pyranosyl acetates)
     533-67-5, 2-Deoxy-D-ribose
ΙT
     RL: PROC (Process)
        (conversion of, to benzoylfuranosyl and -pyranosyl acetates)
     20838-22-6P 20963-97-7P 35898-30-7P
                                           51549-15-6P
ΙT
                                                                130703-07-0P
                                 119933-37-8P
                   66048-53-1P
                                                 119933-40-3P
     59921-49-2P
                    130703-09-2P
                                    130703-10-5P 130703-11-6P
     130703-08-1P
                                                 130703-15-0P
                                 130703-14-9P
     130703-12-7P 130703-13-8P
                    130703-17-2P
                                    130703-18-3P
     130703-16-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (prepn. and ammonolysis of)
                  51255-12-0P
                                 130794-93-3P
IT
     6974-32-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and regioselective condensation of, with silylated purines or
        pyrimidines, nucleosides from)
     50-89-5P, Thymidine, preparation
                                         58-61-7P, Adenosine,
IT
                   118-00-3P, Guanosine, preparation 951-77-9P
     preparation
                             3413-66-9P 4449-40-5P 4449-43-8P
     958-09-8P
                 961-07-9P
                                              13091-57-1P
                                                           15398-66-0P
                  7697-49-6P
                                13091-56-0P
     5682-25-7P
                                                 103216-96-2P
                                                                130703-19-4P
                                  103216-95-1P
     17434-50-3P
                   19916-78-0P
     130703-20-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
     20963-97-7P 35898-30-7P 130703-11-6P
ΙT
     130703-13-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
     (prepn. and ammonolysis of) 20963-97-7 HCAPLUS
RN
     Cytidine, 2'-deoxy-, 3',5'-dibenzoate (8CI, 9CI) (CA INDEX NAME)
CN
Absolute stereochemistry.
```

RN 35898-30-7 HCAPLUS CN Thymidine, 3',5'-dibenzoate (6CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 130703-11-6 HCAPLUS CN 2(1H)-Pyrimidinone, 4-amino-1-(3,5-di-O-benzoyl-2-deoxy-.alpha.-D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 130703-13-8 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(3,5-di-O-benzoyl-2-deoxy-.alpha.-D-erythro-pentofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

IT 50-89-5P, Thymidine, preparation 951-77-9P 4449-40-5P 4449-43-8P

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 951-77-9 HCAPLUS

CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 4449-40-5 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-.alpha.-D-erythro-pentofuranosyl)(9CI) (CA INDEX NAME)

RN 4449-43-8 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-.alpha.-D-erythro-pentofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1990:631914 HCAPLUS

DN 113:231914

TI A simple method for the solid phase synthesis of oligodeoxynucleotides containing O4-alkylthymine

AU Xu, Yao Zhong; Swann, Peter F.

CS Dep. Biochem., Univ. Coll., London, WC1E 6BT, UK

SO Nucleic Acids Research (1990), 18(14), 4061-5

CODEN: NARHAD; ISSN: 0305-1048

DT Journal

LA English

CC 33-9 (Carbohydrates)

AB A route to prep. the cyanoethyl phosphoramidite monomer of O4-alkylthymine and a method for the routine solid-phase synthesis of oligodeoxynucleotides contg. O4-alkylthymine are described. This method was used to make DNA sequences up to 48 bases in length. The amino function of the adenine and guanine in the sequence were protected with the phenoxyacetyl group, and that of cytosine with the isobutyryl group. The phosphodiesters were protected with the cyanoethyl group. This allowed complete deprotection of the oligomer with alkoxide ions (methanol/1,8- diazabicyclo[5.4.0]undec-7-ene (DBU) for the oligomers contg. O4-methylthymine, or ethanol/DBU for those contg. O4-ethylthymine) attack the O4-alkylthymine to form 5-methylcytosine. There was no detectable loss of the alkyl group to form thymine.

oligodeoxynucleotide solid phase synthesis; thymidine oxygen alkylated prepn phosphorylation; phosphorylation alkylthymidine ethylthymidine methylthymidine; alkylthymidine phosphoramidite prepn oligomerization; ethylthymidine phosphoramidite prepn oligomerization; methylthymidine phosphoramidite prepn oligomerization; oligomerization alkylthymidine

ethylthymidine methylthymidine phosphoramidite

IT Nucleotides, preparation

```
RL: SPN (Synthetic preparation); PREP (Preparation)
        (O-alkylthymidine phosphoramidates, prepn. of, as monomers for
        oligonucleotide synthesis)
ΙT
     Nucleosides, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (O-alkylthymidines, phosphorylation of, with
        chloro(cyanoethoxy) (diisopropylamino) phosphine)
IT
     Nucleosides, preparation
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (O-alkylthymidines, prepn. of, as precursors of oligonucleotide
        monomers)
ΙT
     Nucleotides, polymers
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oligo-, deoxy-, solid phase synthesis of, using O-alkylthymidine
        phosphoramidates)
ΙT
     Nucleotides, polymers
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oligo-, deoxyribo-, solid phase synthesis of, using O-alkylthymidine
        phosphoramidates)
ΙT
     117775-85-6P
                     117775-90-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and phosphorylation of, with chloro(cyanoethoxy) (diisopropylami
        no)phosphine)
IT
     50591-13-4P, O4-Methylthymidine
                                      59495-22-6P, O4-Ethylthymidine
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and tritylation of, with dimethoxytrityl chloride)
IT
     130583-06-1P
                    130583-07-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, as oligonucleotide monomer for solid phase synthesis)
IT
     80991-40-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn., alkoxylation, and desilylation of)
IT
     40733-26-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (prepn., chlorination, and amination of, with imidazole)
     50-89-5, Thymidine, reactions
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (silylation of)
     130583-08-3P
IΤ
                    130583-09-4P
                                   130583-10-7P
                                                   130583-11-8P
                                                                  130583-12-9P
     130583-13-0P
     RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
        (solid phase synthesis of, using O-alkylthymidines)
TΥ
     80991-40-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn., alkoxylation, and desilylation of)
RN
     80991-40-8 HCAPLUS
CN
     2(1H) -Pyrimidinone, 1-[2-deoxy-3, 5-bis-0-[(1,1-bis-0-1)]
     dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-5-methyl-4-
     (1H-1,2,4-triazol-1-yl)-(9CI) (CA INDEX NAME)
Absolute stereochemistry.
```

ΙT 40733-26-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

RN

(prepn., chlorination, and amination of, with imidazole) 40733-26-4 HCAPLUS
Thymidine, 3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) CN (CA

INDEX NAME)

Absolute stereochemistry.

IT

50-89-5, Thymidine, reactions RL: RCT (Reactant); RACT (Reactant or reagent)

(silylation of)

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

```
ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2003 ACS
L75
     1989:633480 HCAPLUS
ΑN
DN
     111:233480
     Preparation of cytosine derivatives
ΤI
     Ikeda, Takao
IN
     Yamasa Shoyu Co., Ltd., Japan
PΑ
     Jpn. Kokai Tokkyo Koho, 5 pp.
SO
     CODEN: JKXXAF
DT
     Patent
LA
     Japanese
     ICM C07H019-06
IC
     33-9 (Carbohydrates)
CC
     Section cross-reference(s): 28
FAN.CNT 1
                                                            DATE
                                           APPLICATION NO.
     PATENT NO.
                      KIND
                            DATE
                                           _____
                            _____
                                           JP 1987-302889
                                                            19871130 <--
                      A2
                            19890606
PΙ
     JP 01143892
                            19951108
     JP 07103149
                       B4
PRAI JP 1987-302889
                            19871130 <--
     MARPAT 111:233480
OS
GΙ
```

RN

69-74-9 HCAPLUS

The title derivs. I (R1 = H, halo, alkyl; R2 = sugar residue), were prepd. AΒ in high yield by treating uracils II (R1 = same as I, R3 = sugar residue whose OHs were protected) with imidazole (III) in the presence of phosphates, then aminating the resulting imidazolylpyrimidinones (IV). Thus, 2'-deoxyuridine diacetate was stirred with III in the presence of Et3N and (PhO)2POC1 at 90.degree. for 1 day, treated with aq. . NH3, then treated with conc. HCl to give 93% 2'-deoxycytidine-HCl. cytosine sugar; cytidine; uracil substitution imidazole ST 69-74-9P, 1-(.beta.-D-Arabinofuranosyl)cytosine hydrochloride ΙT 3992-42-5P 7244-51-1P, Cytidine hydrochloride 123931-03-3P, 2',3'-Dideoxycytidine hydrochloride RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by substitution of uracils with imidazole) 288-32-4, Imidazole, reactions IT RL: RCT (Reactant); RACT (Reactant or reagent) (substitution by, of uracils) 2524-64-3, Diphenyl chlorophosphate ΙT RL: RCT (Reactant); RACT (Reactant or reagent) (substitution of uracils with imidazole in presence of) 4105-38-8 13030-62-1 14057-18-2, ΙT 1-(2',3',5'-O-Triacetyl-.beta.-D-arabinofuranosyl)uracil RL: RCT (Reactant); RACT (Reactant or reagent) (substitution reaction of, with imidazole) 69-74-9P, 1-(.beta.-D-Arabinofuranosyl)cytosine hydrochloride ΙT 3992-42-5P 7244-51-1P, Cytidine hydrochloride RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by substitution of uracils with imidazole)

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### HCl

RN 3992-42-5 HCAPLUS

CN Cytidine, 2'-deoxy-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

# ● HCl

RN 7244-51-1 HCAPLUS

CN Cytidine, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ● HCl

RN 4105-38-8 HCAPLUS

CN Uridine, 2',3',5'-triacetate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 13030-62-1 HCAPLUS

CN Uridine, 2'-deoxy-, 3',5'-diacetate (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 14057-18-2 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2,3,5-tri-O-acetyl-.beta.-D-arabinofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1989:439791 HCAPLUS

DN 111:39791

TI The oxidative chlorination of pyrimidine and purine bases, and nucleosides using acyl chloride-dimethylformamide-m-chloroperbenzoic acid system

AU Ryu, E. K.; Kim, J. N.

CS Div. Org. Chem., Korea Res. Inst. Chem. Technol., Daedeog-Danji, 300-31, S. Korea

SO Nucleosides & Nucleotides (1989), 8(1), 43-8 (CODEN: NUNUD5; ISSN: 0732-8311

DT Journal

LA English

CC 33-9 (Carbohydrates)

```
Section cross-reference(s): 28
OS
     CASREACT 111:39791
     Pyrimidine and purine bases, and nucleosides were chlorinated by the
AB
     reaction of acyl chloride in DMF with MCPBA under mild conditions in
     moderate yields.
     oxidative chlorination pyrimidine purine nucleoside; acyl chloride
ST
     oxidative chlorination
TΨ
     Chlorination
         (of pyrimidine and purine bases and nucleosides using acyl
        chloride-dimethylformamide-chloroperbenzoic acid system)
TΤ
     Acid chlorides
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (oxidative chlorination of pyrimidine and purine bases and nucleosides
        with DMF, chloroperbenzoic acid, and)
ΙT
     Nucleosides, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (purine, oxidative chlorination of, using acyl chloride
        dimethylformamide-chloroperbenzoic acid system)
IT
     Nucleosides, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (pyrimidine, oxidative chlorination of, using acyl chloride
        dimethylformamide-chloroperbenzoic acid system)
IT
     98-88-4, Benzoyl chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidative chlorination of pyrimidine and purine bases and nucleosides
        using DMF, chloroperbenzoic acid, and)
     75-36-5, Acetyl chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidative chlorination of uracil by chloroperbenzoic acid and)
     120-73-0D, Purine, bases and nucleosides 289-95-2D, Pyrimidine, bases
ΙT
     and nucleosides
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidative chlorination of, using acyl chloride-dimethylformamide-
        chloroperbenzoic acid system)
TΤ
     58-61-7, Adenosine, reactions 58-96-8, Uridine 65-46-3
     , Cytidine
                  66-22-8, 2,4(1H,3H)-Pyrimidinedione, reactions
     73-24-5, 1H-Purin-6-amine, reactions 951-77-9
     951-78-0
                958-09-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidative chlorination of, with acyl chloride-dimethylformamide-
        chloroperbenzoic acid system)
ΙT
     50-90-8P
              1820-81-1P
                             2347-43-5P 2880-89-9P
     25130-29-4P
                   28128-28-1P 32387-56-7P 34408-14-5P
     69260-67-9P
                   85562-55-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
IΤ
     58-96-8, Uridine 65-46-3, Cytidine 951-77-9
     951-78-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidative chlorination of, with acyl chloride-dimethylformamide-
        chloroperbenzoic acid system)
     58-96-8 HCAPLUS
RN
     Uridine (8CI, 9CI) (CA INDEX NAME)
```

RN 65-46-3 HCAPLUS CN Cytidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 951-77-9 HCAPLUS CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 951-78-0 HCAPLUS CN Uridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 50-90-8P 2880-89-9P 25130-29-4P
 32387-56-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) RN

50-90-8 HCAPLUS Uridine, 5-chloro-2'-deoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN 2880-89-9 HCAPLUS

Uridine, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN 25130-29-4 HCAPLUS

Cytidine, 5-chloro- (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

32387-56-7 HCAPLUS RN

Cytidine, 5-chloro-2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME) CN

JP 1994-119539

JP 1996-221531

US 1991-780346

US 1991-780347

US 1992-981148

US 1993-981026

US 1994-181358

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ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2003 ACS
T.75
AN
     1988:493540 HCAPLUS
DN
     109:93540
ΤI
     Preparation of (aminoalkynyl) nucleotides as intermediates for fluorescent
     chain terminators for DNA sequencing
IN
     Hobbs, Frank Worden, Jr.; Cocuzza, Anthony Joseph
PA
     du Pont de Nemours, E. I., and Co., USA
SO
     Eur. Pat. Appl., 40 pp.
     CODEN: EPXXDW
DT
     Patent
LA
     English
IC
     ICM C07D403-04
          C07D471-04; C07H019-14; C07H019-073; C07D239-54
ICI
     C07D471-04, C07D239-00, C07D209-00
     33-9 (Carbohydrates)
     Section cross-reference(s): 9
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                                                              _____
     EP 251786
PΙ
                       Α2
                             19880107
                                            EP 1987-305844
                                                              19870701 <--
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                             19891206
     EP 251786
                       В1
                             19941130
         R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
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                                            US 1987-57565
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                                                              19870701 <--
     NO 171981
                       В
                             19930215
     NO 171981
                       С
                             19930526
     ES 2066760
                       Т3
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                                            JP 1987-166224
                                                              19870702 <--
     JP 08005908
                       В4
                             19960124
     JP 09124636
                                            JP 1996-221531
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                             19970513
                                                              19870702 <--
     JP 10158530
                       Α2
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                             19980616
                                            US 1991-713906
                                                              19910612 <--
     US 5151507
                       Α
                             19920929
     DK 9300819
                                            DK 1993-819
                       Α
                                                              19930707 <--
                             19930707
     DK 9300820
                                            DK 1993-820
                                                              19930707 <--
                       Α
                             19930707
     US 5625081
                             19970429
                                            US 1994-181284
                       Α
                                                              19940113 <---
                                                              19940207 <--
     US 5558991
                             19960924
                                            US 1994-192915
                       Α
     US 5608063
                             19970304
                                            US 1995-412409
                                                              19950328 <--
                       Α
PRAI US 1986-881372
                             19860702
                                       <--
     US 1987-57565
                             19870612
                                       <--
     US 1987-57566
                             19870612
                                       <--
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19870702

19870702

19911022

19911022

19921124

19930217

19940113

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
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The title compds. [I-IV; R = H, NH2; R1 = R2R3NZC.tplbond.C; R2, R3 = H,
C1-4 alkyl, protecting group; R4 = sugar moiety Q, Q1, ether moiety Q2; R5
= H, (HO)2P(O), H3P2O6, H4P3O9; when R7 = R8 = H, then R6 = H, OH, F, NH2,
N3; when R7 = H, R8 = OH, then R6 = H, OH; when R7 = OH, R8 = H, then R6 =
OH; Z = diradical moiety of 1-20 atoms] and their salts were prepd. for
coupling with fluorescent dyes to prep. fluorescent chain terminators for
DNA sequencing. 6-Methoxy-2-(methylthio)-9-(2,3-dideoxy-5-O-trityl-.beta.-
D-ribofuranosyl)-7-deazapurine, prepd. in 5 steps from
6-methoxy-2-(methylthio)-7-deazapurine, was iodinated by treatment with
N-iodosuccinimide and the 7-iodo deriv. was de-0-methylated, oxidized to
the sulfoxide and ammonolyzed, and detritylated to give azaguanosine IV (R
= NH2, R1 = iodo, R4 = Q, R5-R8 = H). This was coupled with
HC.tplbond.CCH2NHCOCF3 in the presence of (Ph3P)4Pd/CuI catalyst and the
product converted to the triphosphate and deprotected to give IV (R = NH2,
R1 = H2NCH2C.tplbond.C, R4 = Q, R5 = H4P3O9, R6-R8 = H). This was
condensed with a xanthene deriv. (prepn. given) to give fluorescent chain
terminator V.
```

ST aminoalkynylnucleotide intermediate chain terminator DNA sequencing; nucleotide aminoalkynyl; fluorescent chain terminator DNA sequencing

IT Coupling reaction catalysts

(cuprous iodide and palladium phosphine complexes, for iodonucleoside bases with alkynylamines)

IT Deoxyribonucleic acid sequences

(detn. of, (aminoalkynyl)nucleotides as intermediates for fluorescent chain terminators for)

IT Nucleotides, preparation

RL: SPN (Synthetic preparation); PREP (Preparation) (deoxyribo-, aminoalkynyl-, prepn. of, as intermediates for fluorescent chain terminators for DNA sequencing)

IT 516-12-1, N-Iodosuccinimide 7790-99-0, Iodine monochloride RL: RCT (Reactant); RACT (Reactant or reagent) (iodination by, of nucleoside bases)

IT 14719-21-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and coupling of, with iodonucleosides, catalysts for)

IT 115899-58-6P

IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as fluorescent chain terminator for DNA sequencing)

496-73-1P **611-53-0P** 634-65-1P 6248-20-0P 15252-44-5P, 18202-10-3P, 11-Dodecyn-1-ol 4-Pentyn-1-amine 40627-30-3P 54384-05-3P 64702-16-5P 71084-07-6P 88499-44-9P 96027-44-0P 97337-37-6P 97481-18-0P 98891-39-5P 98891-40-8P 98921-75-6P 105784-83-6P 114748-39-9P 114748-40-2P 114748-41-3P 114748-42-4P 114748-43-5P 114748-44-6P 114748-45-7P 114748-46-8P 114748-47-9P 114748-49-1P 114748-48-0P 114748-50-4P 114748-51-5P 114748-52-6P 114748-53-7P 114748-54-8P 114748-55-9P 114748-56-0P 114748-57-1P 114748-58-2P 114748-59-3P 114748-60-6P 114748-61-7P 114748-62-8P 114748-64-0P 114748-63-9P 114748-65**-**1P 114748-66-2P 114748-67-3P 114748-69-5P 114748-68-4P 114748-70-8P 114748-71-9P 114748-73-1P 114748-76-4P 115899-24-6P 115899-25-7P 115899-26-8P 115899-27-9P 115899-28-0P 115899-29-1P 115899-30-4P 115899-31-5P 115899-32-6P 115899-33-7P 115899-34-8P 115899-35-9P 115899-36-0P 115899-37-1P 115899-38-2P 115899-39-3P 115899-40-6P 115899-41-7P 115899-42-8P 115899-43-9P 115899-44-0P 115899-45-1P 115899-46-2P 115899-47-3P 115899-48-4P 115899-49-5P 115899-50-8P 115899-51-9P 115899-52-0P 115899-57-5P 115899-54-2P 115899-55-3P 115899-56-4P 115899-53-1P 115920-24-6P 115944-91-7P 115920-25-7P 115899-59-7P 115899-60**-**0P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as fluorescent chain terminator intermediate, for DNA sequencing) 69-33-0, Tubercidin 54-42-2, 5-Iodo-2'-deoxyuridine 93-61-8. 95-01-2, 2,4-Dihydroxybenzaldehyde 102-82-9 N-Methylformanilide

ΙT 108-30-5, Succinic anhydride, reactions 108-46-3, Resorcinol, reactions 354-38-1, 2,2,2-Trifluoroacetamide 431-47-0, Methyl trifluoroacetate 608-25-3, 2-Methylresorcinol 951-77-9, 2'-Deoxycytidine 2450-71-7, Propargylamine 3601-89-6 5983-09-5 6066-82-6, 6867-30-7 7481-89-2, 2',3'-Dideoxycytidine N-Hydroxysuccinimide 13464-19-2, Phenyl 7722-88-5, Tetrasodium pyrophosphate 29877-76-7 chlorothioformate 14267-92-6, 5-Chloro-1-pentyne 68724-12-9, 1-[(2-54384-06-4 40635-67-4 51795-88-1 91713-43-8 91713-44-9 Hydroxyethoxy) methyl] cytosine RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, in prepn. of fluorescent chain terminators for DNA

IT 611-53-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as fluorescent chain terminator intermediate, for DNA
 sequencing)

RN 611-53-0 HCAPLUS

CN Cytidine, 2'-deoxy-5-iodo- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

sequencing)

IT 54-42-2, 5-Iodo-2'-deoxyuridine 951-77-9,

2'-Deoxycytidine

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in prepn. of fluorescent chain terminators for DNA sequencing)

RN 54-42-2 HCAPLUS

CN Uridine, 2'-deoxy-5-iodo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

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951-77-9 HCAPLUS
RN
CN
     Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)
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Absolute stereochemistry. Rotation (+).

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ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2003 ACS 1988:112894 HCAPLUS
L75
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ΑN

DN 108:112894

Pyridopyrimidine nucleotide derivatives ΤI

Inoue, Hideo; Ohtsuka, Eiko; Imura, Akihiro; Masuda, Kenichi; Kamimura, ΙN Takashi

PΑ Teijin Ltd. , Japan

PCT Int. Appl., 51 pp. SO

CODEN: PIXXD2

DT Patent

LA French

IC ICM C07H019-04 ICS C07H021-00

G01N021-75; G01N033-50; G01N033-58; G01N033-68; C12Q001-68; C12N015-00 ICA

CC 33-9 (Carbohydrates)

Section cross-reference(s): 1, 9

FAN	.CNT	1
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FAN.CNT 1						
	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
ΡI	WO 8701373	A1	19870312		WO 1986-JP441	19860828 <
	W: JP, US					
	RW: CH, DE,	FR, GB				
	EP 235301	A1	19870909		EP 1986-905396	19860828 <
	EP 235301	В1	19920722			
	R: CH, DE,	FR, GB	, LI			
	JP 07025788	B4	19950322		JP 1986-504618	19860828 <
	US 4965350	A	19901023		US 1989-351317	19890511 <
PRAI	JP 1985-197689		19850909	<		
	WO 1986-JP441	•	19860828	<		
	US 1987-54910		19870511	<		
GI						

AB Fluorescent pyridopyrimidine nucleotide derivs. [I; X1, Y1 = HO[P(O)(OH)O]n, where n = 0-3; however, n cannot be 0 for both X1 and Y1; Z1 = HO[P(O)(OH)O]m, where m = 0-3; W1 = H, OH; when R1 = amino, halo, R1R2 = bond; when R2 = H, a1ky1, R1 = O] and II [X2 = HO[P(O)(OH)O].dwnarw.r (r = 0-3), etc.; Y2, Z2 = O, H, OH, etc.; W2 = H,OH] are prepd. for DNA probes. 3-.beta.-D-Deoxyribofuranosyl-2,7dioxopyrido[2,3-d]pyrimidine (III, R3 = H) in (EtO)3P(O) was treated with POC13 at 0.degree. for 6 h to give, after hydrolysis, the 5'-phosphate [III, R3 = (HO)2P(O)], which was condensed with the appropriate nucleotides by the solid-phase method to give dodecanucleotides, e.g.,  $dGGGAAFTTTCCC\ (F = fluorescent nucleotide)$ , which were useful as DNA probes. pyridopyrimidine nucleotide deriv prepn DNA probe; fluorescent

ST pyridopyrimidine nucleotide deriv

ΙT Deoxyribonucleic acids

RL: RCT (Reactant); RACT (Reactant or reagent)

(probe, synthesis of fluorescent oligonucleotides for)

IT 65-46-3 951-77-9

RL: PROC (Process)

(conversion of, into cytidinylmercury chloride)

ΙT 107-13-1, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyanovinylation by, of iododeoxyuridine)

ΙT 54-42-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyanovinylation of)

IT 96-33-3D, palladium complex 7440-05-3D, Me acrylate complex RL: RCT (Reactant); RACT (Reactant or reagent) (methoxycarbonylvinylation by, of cytidinylmercury chloride)

IT 96-33-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(methoxycarbonylvinylation by, of iododeoxyuridine)

ΙT 80173-35-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and acetylation of)

113295-55-9P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and amination of)

ΙŢ 113295-52-6P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

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(prepn. and chlorination of)
TT.
     113295-53-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and deacetylation of)
IT
     65523-07-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and methoxycarbonylvinylation of)
IT
     147-94-4P
                81206-83-9P
                               99517-98-3P
                                             113295-47-9P
     113295-50-4P
                    113295-51-5P
                                   113321-13-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and phosphorylation of)
IT
     81244-97-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and photochem. cyclization of)
ΙT
     113295-56-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and photochem. decyanovinylation of)
     99517-99-4P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction of, with chloro(diisopropylamino)methoxyphosphine)
IT
     99518-04-4P
                   99518-06-6P 99518-08-8P
                                              99533-62-7P
                                                              113295-46-8P
                    113295-49-1P
     113295-48-0P
                                   113295-54-8P
                                                  113295-57-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for DNA probe)
ΙT
     86030-43-5, Chloro(diisopropylamino)methoxyphosphine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with protected deoxyribofuranosyldioxopyridopyrimidine)
ΙT
     65-46-3 951-77-9
     RL: PROC (Process)
        (conversion of, into cytidinylmercury chloride)
RN
     65-46-3 HCAPLUS
CN
     Cytidine (8CI, 9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

RN 951-77-9 HCAPLUS CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 54-42-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyanovinylation of)

RN 54-42-2 HCAPLUS

CN Uridine, 2'-deoxy-5-iodo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 147-94-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and phosphorylation of)

RN 147-94-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1987:637192 HCAPLUS

DN 107:237192

TI Pyridyl groups for protection of the imide functions of uridine and guanosine. Exploration of their displacement reactions for site-specific modifications of uracil and guanine bases

AU Zhou, X. X.; Welch, C. J.; Chattopadhyaya, J.

CS Biomed. Cent., Uppsala Univ., Uppsala, S-751 23, Swed.

SO Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (

```
1986), B40(10), 806-16
     CODEN: ACBOCV; ISSN: 0302-4369
DT
     Journal
LA
     English
CC
     33-9 (Carbohydrates)
OS
     CASREACT 107:237192
AΒ
     For the protection of the O-4 function of uridine and the O-6 of
     quanosine, 2-, 3- and 4-hydroxopyridines, 2-pyridinethiol,
     6-methyl-2-hydroxy- and 6-methyl-3-hydroxypyridines were employed.
     substituted pyridines gave pyridyl-N- and/or pyridyl-O-substituted
     derivs., depending both upon the position of the hydroxyl and Me groups in
     the pyridine ring, at the C-4 and the C-6 of the uracil and quanine
     residues, resp. These groups were good leaving groups for nucleophilic
     substitution reactions by amines, thiolates and oximate. If
     needed, the rate of these substitution reactions could be conveniently
     increased by almost 1000-fold by conversion of the pyridyl moiety to its
     methiodide.
ST
     pyridyl group protection uridine guanosine; nucleophilic substitution
     uridine quanosine
IT
     Substitution reaction, nucleophilic
        (of pyridyl derivs. of uridine and guanosine)
ΙT
     Protective groups
        (substituted pyridyl, for imide functions of uridine and guanosine)
TΤ
     108782-91-8P 111426-23-4P
                                111426-24-5P 111426-25-6P
     111426-26-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and deprotection of)
ΙT
     4105-38-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PRÉP
     (Preparation); RACT (Reactant or reagent)
        (prepn. and reaction of, with pyridine derivs.)
IT
     108324-68-1P
                    108324-69-2P
                                   108324-70-5P
                                                  108324-71-6P
     108324-74-9P
                    108324-75-0P
                                   108324-77-2P
                                                  108324-78-3P
     108324-80-7P
                    108348-48-7P
                                   111426-27-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and substitution reactions of)
ΙT
     10578-79-7P 98222-28-7P
                               99519-13-8P
                                             108324-72-7P
     108324-73-8P 111426-18-7P 111426-19-8P
     111426-20-1P
                    111426-21-2P
                                   111426-22-3P
                                                  111426-28-9P
     111426-29-0P
                    111426-30-3P
                                   111426-31-4P
                                                  111426-32-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
IT
     65-46-3P, Cytidine
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, from uridine)
     85078-95-1P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn., trimethylsilylation, and reaction with pyridine deriv.)
TΤ
     110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions
     506-59-2, Dimethylamine hydrochloride 593-51-1, Methylamine
    hydrochloride
                     5680-79-5, Glycine methyl ester hydrochloride
                                                                      5680-80-8
     37602-52-1
                  86175-49-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with uridine deriv.)
ΙT
                           109-00-2, 3-Pyridinol
     108-96-3, 4-Pyridone
                                                    142-08-5, 2-Pyridone
     1121-78-4, 6-Methyl-3-pyridinol
                                       2637-34-5
                                                   3279-76-3,
     6-Methyl-2-pyridone
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with uridine or guanosine derivs.)
ΙT
     69304-38-7
```

RL: RCT (Reactant); RACT (Reactant or reagent)

(trimethylsilylation of, for reaction with substituted pyridines)

ΙT 58-96-8, Uridine

RL: RCT (Reactant); RACT (Reactant or reagent) (O-acetylation of)

IT 111426-23-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (prepn. and deprotection of)

111426-23-4 HCAPLUS RN

2(1H)-Pyrimidinone, 4-(2-oxo-1(2H)-pyridinyl)-1-.beta.-D-ribofuranosyl-CN

Absolute stereochemistry.

ΙT 4105-38-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with pyridine derivs.) 4105-38-8 HCAPLUS

RN

Uridine, 2',3',5'-triacetate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

IT108324-74-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (prepn. and substitution reactions of)

108324-74-9 HCAPLUS RN

2(1H)-Pyrimidinone, 4-(4-oxo-1(4H)-pyridinyl)-1-(2,3,5-tri-0-acetyl-.beta.-CN

IT 10578-79-7P 98222-28-7P 108324-73-8P 111426-18-7P 111426-19-8P 111426-20-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 10578-79-7 HCAPLUS

CN Cytidine, N-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 98222-28-7 HCAPLUS

CN Cytidine, N, N-dimethyl-, 2', 3', 5'-triacetate (7CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 108324-73-8 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(2-oxo-1(2H)-pyridinyl)-1-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

RN 111426-18-7 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(1-piperidinyl)-1-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111426-19-8 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(4-morpholinyl)-1-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111426-20-1 HCAPLUS

CN Cytidine, N-methyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

IT **65-46-3P**, Cytidine

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, from uridine)

RN 65-46-3 HCAPLUS

CN Cytidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT **58-96-8**, Uridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(O-acetylation of)

RN 58-96-8 HCAPLUS

CN Uridine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1987:534617 HCAPLUS

DN 107:134617

TI Hybridization triggered cross-linking of deoxyoligonucleotides

AU Webb, Thomas R.; Matteucci, Mark D.

CS Dep. Mol. Biol., Genentech, Inc., San Francisco, CA, 94080, USA

SO Nucleic Acids Research (1986), 14(19), 7661-74

CODEN: NARHAD; ISSN: 0305-1048

DT Journal

LA English

CC 33-10 (Carbohydrates)

Section cross-reference(s): 6

```
AΒ
      Oligodeoxynucleotides contg. the modified base 5-methyl-N4,N4-
      ethanocytosine (Ce) were prepd. on polymer support. The
      9-fluorenylmethoxycarbonyl group was used as a protecting group for the
      exocyclic amines of dA and dC. This group can be removed
      rapidly under very mild conditions. Óligomers contg. the Ce base form a
      cross-link when hybridized to their complementary deoxyoligonucleotides.
      Some of the scope and limitations of these cross-link forming
      oligonucleotides are reported.
      deoxyoligonucleotide prepn hybridization crosslinking; nucleotide
      oligodeoxy prepn hybridization crosslinking; ethanocytosine
      oligodeoxynucleotide; protective group fluorenylmethoxycarbonyl nucleotide
 IT
      Crosslinking
         (of deoxyoligonucleotides, hybridization triggered)
 ΙT
      Protective groups
         ((fluorenylmethoxy)carbonyl, for exocyclic amino group of
         deoxyadenosine and deoxycytidine, in synthesis of
         oligodeoxynucleotides)
 ΙT
      Nucleotides, polymers
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (oligo-, deoxy-, hybridization triggered cross-linking of)
 ΙT
      Nucleotides, polymers
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (oligo-, deoxyribo-, prepn. of, contg. methylethanocytosine)
      951-77-9, 2'-Deoxycytidine
 ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         ((fluorenylmethoxy)carbonylation and dimethoxytritylation of, for
         synthesis of oligodeoxynucleotides)
ΤT
      87424-19-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. and dimethoxytritylation of, for synthesis of
         oligodeoxynucleotides)
ΙT
     80991-40-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. and reaction of, with aminoethanol)
ΙT
     109389-24-4P 109389-25-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and reaction of, with aziridine)
IT
     110071-17-5P
                    110341-91-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and reaction of, with deoxyoligonucleotides)
TΤ
     109489-08-9P
                    109489-09-0P
                                   109489-10-3P
                                                   109489-11-4P
                                                                  109489-12-5P
     109489-13-6P
                    109489-14-7P
                                    109489-15-8P
                                                   109489-16-9P
                                                                  109489-17-0P
     109489-18-1P
                    109523-81-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction of, with oligodeoxynucleotide contg. modified base
        methylethanocytosine)
ΙT
     101712-10-1P
                   109389-29-9P 109389-31-3P
                                                  109489-06-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
     109389-26-6P 109389-27-7P 109389-28-8P
ΙT
     109389-32-4P
                   109389-33-5P
                                  109420-85-1P
                                                  109420-86-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for synthesis of oligodeoxynucleotides)
ΙT
     50-89-5, Thymidine, reactions 951-78-0, 2'-Deoxyuridine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with (dimethylamino)trimethylsilane and phosphoryl
        tristriazolide)
ΙT
     72741-18-5
```

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with deoxyribonucleosides)

ΙT 40733-26-4 109389-30-2 98796-51-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with phosphoryl tristriazolide)

ΙT 141-43-5, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with triazolyldeoxyribonucleoside)

IT 151-56-4, Aziridine, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with triazolyldeoxyribonucleosides)

IT 951-77-9, 2'-Deoxycytidine

RL: RCT (Reactant); RACT (Reactant or reagent)

((fluorenylmethoxy)carbonylation and dimethoxytritylation of, for synthesis of oligodeoxynucleotides)

RN 951-77-9 HCAPLUS

CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

#### ΙT 80991-40-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with aminoethanol) 80991-40-8 HCAPLUS

RN

CN 2(1H)-Pyrimidinone, 1-[2-deoxy-3,5-bis-0-[(1,1-

dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-5-methyl-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### ΙT 109389-24-4P 109389-25-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepri. and reaction of, with aziridine)

RN 109389-24-4 HCAPLUS CN 2(1H)-Pyrimidinone, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 109389-25-5 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-5-methyl-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 109389-26-6P 109389-27-7P 109389-28-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, for synthesis of oligodeoxynucleotides)

RN 109389-26-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(1-aziridinyl)-1-[2-deoxy-3,5-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-5-methyl-(9CI) (CA INDEX NAME)

RN 109389-27-7 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(1-aziridinyl)-1-(2-deoxy-.beta.-D-erythropentofuranosyl) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

109389-28-8 HCAPLUS RN

CN 2(1H)-Pyrimidinone, 4-(1-aziridinyl)-1-(2-deoxy-.beta.-D-erythropentofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ΙT

50-89-5, Thymidine, reactions 951-78-0, 2'-Deoxyuridine RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with (dimethylamino)trimethylsilane and phosphoryl tristriazolide)

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

RN 951-78-0 HCAPLUS

CN Uridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 40733-26-4

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phosphoryl tristriazolide)

RN 40733-26-4 HCAPLUS

CN Thymidine, 3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1987:214307 HCAPLUS

DN 106:214307

TI Conversion of uracil derivatives to cytosine derivatives

IN Kawada, Mitsuru; Matsumoto, Kiyoharu; Tsurushima, Masaaki

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW DTPatent LA English IC ICM C07H019-06 CC 33-9 (Carbohydrates) FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_\_ -----PΙ EP 204264 A2 19861210 EP 1986-107302 19860529 <--EP 204264 Α3 19880107 EP 204264 B1 19900816 R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE JP 62089667 A2 19870424 JP 1986-24640 19860205 <--US 4754026 Α 19880628 US 1986-866960 19860527 <--AT 55609 Ε 19900915 AT 1986-107302 19860529 <--CN 86103615 Α 19861203 CN 1986-103615 19860601 <--CN 1012367 В 19910417 ES 555646 A1 19871201 ES 1986-555646 19860603 <--CA 1268174 A1 19900424 CA 1986-510679 19860603 <--ES 557707 A1 19880301 ES 1987-557707 19870901 <--PRAI JP 1985-121786 19850604 <---JP 1986-24640 19860205 <---EP 1986-107302 19860529 <--OS CASREACT 106:214307 GΙ

O-Sulfonated uracils I (R1 = H, alkyl, alkoxy, halo; R2 = protected glycosyl; R3SO2 = org. sulfonyl group) were prepd. by treating the corresponding protected uracils with R3SO2X (X = halo) in an org. solvent at 0-150.degree. in the presence of K2CO3. Aminolysis of I with NH3 or primary amines gave cytosines, intermediates for pharmaceuticals such as citicoline (no data). 2',3',5'-Tri-O-acetyluridine was stirred at 80.degree. in MeCOCH2CHMe2 with 4-MeC6H4SO2Cl and K2CO3 to give 97.7% I (R1 = H, R2 = 2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl, R3 = 4-MeC6H4). This was allowed to stand overnight at room temp. in MeOH/concd. aq. NH3 to give 91.4% cytidine (II).

ST uridine sulfonylation aminolysis; phenylsulfonyluracil aminolysis; cytidine

IT 64-04-0, Phenethylamine 123-75-1, Pyrrolidine, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (aminolysis by, of O-sulfonylated uridine deriv.)

IT 7664-41-7, Ammonia, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

```
(aminolysis by, of O-sulfonylated uridines)
  ΙT
       108273-53-6P
                    108273-54-7P
                                    108273-55-8P
                                                    108273-56-9P
                                                                   108273-57-0P
       108273-58-1P
                     108273-59-2P
                                     108273-60-5P
                                                    108273-61-6P
      RL: SPN (Synthetic preparation); PREP (Preparation)
                                                                   108273-62-7P
          (prepn. and aminolysis-deprotection of)
 IT
      147-94-4P
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of, by sulfonylation-aminolysis of arabinofuranosyluracil
         deriv.)
      65-46-3P, Cytidine 951-77-9P, 1-(2'-Deoxy-.beta.-D-
 IT
      ribofuranosyl)cytosine 2140-61-6P, 5-Methylcytidine
      2341-22-2P, 5-Fluorocytidine 29834-86-4P,
      N, N-Tetramethylenecytidine 108273-51-4P, N-(2-Phenylethyl) cytidine
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by sulfonylation-aminolysis of uridine deriv.)
      98-68-0, 4-Methoxybenzenesulfonyl chloride 773-64-8,
      2,4,6-Trimethylbenzenesulfonyl chloride 6553-96-4, 2,4,6-
      Triisopropylbenzenesulfonyl chloride 52499-94-2,
      Pentamethylbenzenesulfonyl chloride
                                            55661-08-0, 4-Methoxy-2,6-
      dimethylbenzenesulfonyl chloride
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (O-acylation by, of protected uridine deriv.)
     80745-07-9, 4-Methoxy-2,3,6-trimethylbenzenesulfonyl chloride
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (O-acylation by, of protected uridines)
     4105-38-8, 2',3',5'-Tri-O-acetyluridine 4336-39-4,
ΙT
     2',3',5'-Tri-O-acetyl-5-methyluridine 13030-62-1,
     1-(3',5'-Di-O-acetyl-2'-deoxy-.beta.-D-ribofuranosyl)uridine
     14057-18-2, 1-(2',3',5'-Tri-O-acetyl-.beta.-D-
     arabinofuranosyl)uracil 55474-11-8, 2',3',5'-Tri-O-acetyl-5-
     fluorouridine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-sulfonylation of)
ΙT
     147-94-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by sulfonylation-aminolysis of arabinofuranosyluracil
        deriv.)
RN
     147-94-4 HCAPLUS
     2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl- (9CI) (CA INDEX
CN
Absolute stereochemistry.
```

**65-46-3P**, Cytidine **951-77-9P**, 1-(2'-Deoxy-.beta.-D-ΙT ribofuranosyl)cytosine 2140-61-6P, 5-Methylcytidine 2341-22-2P, 5-Fluorocytidine 29834-86-4P, N, N-Tetramethylenecytidine RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by sulfonylation-aminolysis of uridine deriv.) RN 65-46-3 HCAPLUS Cytidine (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN 951-77-9 HCAPLUS CN Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 2140-61-6 HCAPLUS

CN Cytidine, 5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 2341-22-2 HCAPLUS

CN Cytidine, 5-fluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 29834-86-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(1-pyrrolidinyl)-1-.beta.-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 4105-38-8, 2',3',5'-Tri-O-acetyluridine 4336-39-4,
 2',3',5'-Tri-O-acetyl-5-methyluridine 13030-62-1,
 1-(3',5'-Di-O-acetyl-2'-deoxy-.beta.-D-ribofuranosyl)uridine
 14057-18-2, 1-(2',3',5'-Tri-O-acetyl-.beta.-D arabinofuranosyl)uracil 55474-11-8, 2',3',5'-Tri-O-acetyl-5fluorouridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(O-sulfonylation of)

RN 4105-38-8 HCAPLUS

CN Uridine, 2',3',5'-triacetate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 4336-39-4 HCAPLUS CN Uridine, 5-methyl-, 2',3',5'-triacetate (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 13030-62-1 HCAPLUS CN Uridine, 2'-deoxy-, 3',5'-diacetate (8CI, 9CI) (CA INDEX NAME)

RN 14057-18-2 HCAPLUS

2,4(1H,3H)-Pyrimidinedione, 1-(2,3,5-tri-O-acetyl-.beta.-D-CN arabinofuranosyl) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 55474-11-8 HCAPLUS

Uridine, 5-fluoro-, 2',3',5'-triacetate (9CI) CN (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2003 ACS

ΑN 1986:572942 HCAPLUS

105:172942 DN

Syntheses of fluorine containing nuclesides and nucleobases ΤI

Takahara, Takao; Hisanaga, Yorihito ΑU

Daikin Ind., Ltd., Settsu, 566, Japan CS

Nippon Kagaku Kaishi (1985), (10), 2034-9 SO CODEN: NKAKB8; ISSN: 0369-4577

DT Journal

LA Japanese

CC 33-9 (Carbohydrates)

OS CASREACT 105:172942

Reaction of elemental F with the uracil ring systems in AcOH proceeds via AΒ 5,6-difluoro adducts (2 cis-isomers), which were converted to 4 isomer adducts by subsequent solvolysis. Time course adducts were traced by

19F-NMR, but in the case of the cytosine ring systems, the adducts were not detected. The adducts of uridine were converted to stable 6-alkoxy forms and then sepd. 5-Fluorouracil (I), 5-fluorouridine (II), and 2',3'-0-isopropylidene-5'-deoxy-5-fluorouridine (III) were obtained in good yield by fluorination in HF for I and in AcOH for II and III, resp., followed by treatment with HF or an amine. Protected uridines were used as starting materials for II and III. 5-Fluorocytosine and 5-fluorocytidine were also obtained in good yield using HF and AcOH-HF mixt., resp., as a solvent for the fluorination. nucleoside fluorination Nucleosides, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (fluorination of, by hydrofluoric acid or by hydrofluoric acid-acetic acid) Fluorination (of nucleosides and nucleoside bases by hydrofluoric acid or by hydrofluoric acid-acetic acid) 65-46-3 RL: RCT (Reactant); RACT (Reactant or reagent) (fluorination of, by acetic acid-hydrogen fluoride) 66-22-8, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (fluorination of, by hydroflouric acid) 58-96-8 22314-42-7 RL: RCT (Reactant); RACT (Reactant or reagent) (fluorination of, by hydrofluoric acid-acetic acid)

(fluorination of, by hydrofluoric acid-acetic acid)

IT 71-30-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorination of, by hydrogen fluoride)

IT 51-21-8P **316-46-1P** 2022-85-7P **2341-22-2P** 66335-39-5P

IT 65-46-3

ST

IT

ΙT

ΙT

ΙT

RN

RL: RCT (Reactant); RACT (Reactant or reagent) (fluorination of, by acetic acid-hydrogen fluoride) 65-46-3 HCAPLUS

CN Cytidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 58-96-8

RN

RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of, by hydrofluoric acid-acetic acid)
58-96-8 HCAPLUS
Uridine (8CI, 9CI) (CA INDEX NAME)

IT 316-46-1P 2341-22-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

316-46-1 HCAPLUS RN

Uridine, 5-fluoro- (6CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN2341-22-2 HCAPLUS

CNCytidine, 5-fluoro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN1986:497860 HCAPLUS

DN 105:97860

Synthesis of N4-mono- and dialkyl-2'-deoxycytidines and their insertion ΤI into an oligonucleotide

ΑU

Kraszewski, A.; Delort, A. M.; Teoule, R. Dep. Rech. Fond., Cent. Etud. Nucl. Grenoble, Grenoble, F-38041, Fr. CS SO

Tetrahedron Letters (1986), 27(7), 861-4 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LAEnglish

CC 33-9 (Carbohydrates)

OS CASREACT 105:97860

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AB
     Treatment of 3',5'-di-O-acetyl-4-thio-2'-deoxyuridine with mono or
     dialkylamines in EtOH gave 11 title deoxycytidines I (R = MeNH, Me2CHNH,
     Me2N, Et2N, piperidino, etc.). I (R = MeNH) was incorporated into the
     oligonucleotide chain d(CGm4CGCG).
ST
     deoxycytidine alkyl dialkyl; cytidine deoxy alkyl dialkyl; oligonucleotide
     alkyldeoxycytidine; nucleotide oligo alkyldeoxycytidine
IT
     Nucleotides, preparation
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (oligo-, prepn. of, contq. N4-methyldeoxycytidine)
IT
     951-78-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (acetylation of, in synthesis of alkyl deoxycytidines)
     74-89-5, reactions 75-04-7, reactions 75-31-0, reactions
     108-91-8, reactions
                          109-73-9, reactions
                                                109-89-7, reactions
     110-89-4, reactions
                           111-92-2
                                      124-40-3, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (amination by, of thiodeoxyuridine diacetate, in synthesis of
        alkyl deoxycytidine)
ΙT
     103931-23-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and amination of, in synthesis of alkyl
        deoxycytidines)
ΙT
     13030-62-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (prepn. and sulfuration of, in synthesis of alkyl deoxycytidines)
IT
     58927-26-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
IT
     22882-02-6P 53213-03-9P 70465-61-1P
     86811-97-4P 103931-24-4P 103931-25-5P
     103931-26-6P 103931-27-7P 103931-28-8P
     103931-29-9P 103931-30-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, from deoxyuridine)
ΙT
     951-78-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (acetylation of, in synthesis of alkyl deoxycytidines)
     951-78-0 HCAPLUS
RN
CN
     Uridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)
Absolute stereochemistry.
```

IT 13030-62-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. and sulfuration of, in synthesis of alkyl deoxycytidines)

RN 13030-62-1 HCAPLUS

CN Uridine, 2'-deoxy-, 3',5'-diacetate (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 53213-03-9 HCAPLUS CN Cytidine, 2'-deoxy-N, N-dimethyl- (7CI, 9CI) (CA INDEX NAME)

RN 70465-61-1 HCAPLUS CN Cytidine, 2'-deoxy-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 86811-97-4 HCAPLUS CN Cytidine, N-butyl-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 103931-24-4 HCAPLUS CN Cytidine, 2'-deoxy-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 103931-25-5 HCAPLUS CN Cytidine, N-cyclohexyl-2'-deoxy- (9CI) (CA INDEX NAME) Absolute stereochemistry.

RN 103931-26-6 HCAPLUS

CN Cytidine, 2'-deoxy-N-ethyl-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 103931-27-7 HCAPLUS

CN Cytidine, 2'-deoxy-N, N-diethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 103931-28-8 HCAPLUS

CN Cytidine, 2'-deoxy-N, N-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 103931-29-9 HCAPLUS

CN Cytidine, N, N-dibutyl-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 103931-30-2 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1986:168734 HCAPLUS

DN 104:168734

TI Reaction of uracil nucleosides with 1-methylimidazole in the presence of phosphoryl chloride: a convenient method for the synthesis of 4-substituted pyrimidin-2(1H)-one nucleosides

AU Matsuda, Akira; Obi, Kokoh; Miyasaka, Tadashi

CS Sch. Pharm. Sci., Showa Univ., Tokyo, 142, Japan

SO Chemical & Pharmaceutical Bulletin (1985), 33(6), 2575-8 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

CC 33-9 (Carbohydrates)

OS CASREACT 104:168734

GI

## \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Reaction of 2',3',5'-tri-O-benzoyluridine with 1-methylimidazole in the presence of POCl3 in MeCN afforded imidazolium I. Nucleophilic substitutions of I with RH (R = MeO, p-ClC6H4S, EtS, Et2N, CH2:CHCH2NH, and NH2) yielded ribosides II. The method was also successful with 2'-deoxyriboside III (R1 = Me, iodo; R2 = Ac, Bz).

ST benzoyluridine methylimidazole condensation; nucleophilic substitution

methylimidazolylpyrimidinone nucleoside

IT Substitution reaction, nucleophilic

(of (methylimidazolyl)pyrimidinone nucleosides with thiols and amines)

IT Nucleosides, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactions of uracil, with methylimidazole)

IT 1748-04-5 1956-30-5 35898-30-7 98495-56-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(phosphoryl chloride-catalyzed condensation of, with methylimidazole)

IT 616-47-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(phosphoryl chloride-catalyzed condensation of, with tribenzoyluridine)

IT 99679-98-8P 99680-05-4P 99680-07-6P 99692-47-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and imidazolyl substitution of)

IT 2873-31-6P 15049-50-0P **31652-74-1P** 99679-99-9P 99680-00-9P

**99680-01-0P 99680-02-1P** 99680-03-2P 99680-04-3P

99680-06-5P 99680-08-7P

IT 1748-04-5 1956-30-5 35898-30-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(phosphoryl chloride-catalyzed condensation of, with methylimidazole)

RN 1748-04-5 HCAPLUS

CN Uridine, 2',3',5'-tribenzoate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 1956-30-5 HCAPLUS

CN Uridine, 2'-deoxy-5-iodo-, 3',5'-diacetate (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 35898-30-7 HCAPLUS

CN Thymidine, 3',5'-dibenzoate (6CI, 9CI) (CA INDEX NAME)

### IT 99679-98-8P 99680-05-4P 99692-47-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and imidazolyl substitution of)

RN 99679-98-8 HCAPLUS

CN 1H-Imidazolium, 1-[1,2-dihydro-2-oxo-1-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-4-pyrimidinyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• c1-

\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

RN 99680-05-4 HCAPLUS

CN 1H-Imidazolium, 1-[1-(3,5-di-O-acetyl-2-deoxy-.beta.-D-erythro-pentofuranosyl)-1,2-dihydro-5-iodo-2-oxo-4-pyrimidinyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

• c1-

\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*

RN 99692-47-4 HCAPLUS

CN 1H-Imidazolium, 1-[1-(3,5-di-O-benzoyl-2-deoxy-.beta.-D-erythro-pentofuranosyl)-1,2-dihydro-5-methyl-2-oxo-4-pyrimidinyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

C1 -

\*\*\* FRAGMENT DIAGRAM IS INCOMPLETE \*\*\*
IT 31652-74-1P 99680-01-0P 99680-02-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 31652-74-1 HCAPLUS

CN Cytidine, 2',3',5'-tribenzoate (8CI, 9CI) (CA INDEX NAME)

RN 99680-01-0 HCAPLUS

CN Cytidine, N, N-diethyl-, 2', 3', 5'-tribenzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 99680-02-1 HCAPLUS

CN Cytidine, N-2-propenyl-, 2',3',5'-tribenzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1986:82007 HCAPLUS

DN 104:82007

TI Systematic synthesis and biological evaluation of .alpha.— and .beta.—D-xylofuranosyl nucleosides of the five naturally occurring bases in nucleic acids and related analogs

AU Gosselin, Gilles; Bergogne, Marie Christine; De Rudder, Jean; De Clercq, Erik; Imbach, Jean Louis

CS Lab. Chim. Bio-Org., Univ. Sci. Tech. Languedoc, Montpellier, 34060, Fr. SO Journal of Medicinal Chemistry (1986) 29(2) 203-13

Journal of Medicinal Chemistry (1986), 29(2), 203-13 CODEN: JMCMAR; ISSN: 0022-2623

```
Journal
 DT
 LA
      English
 CC
      1-12 (Pharmacology)
      Section cross-reference(s): 33
 GI
 HOCH<sub>2</sub>
    OH
         R^{1}
        ÓН
             Ι
     .alpha.- And .beta.-D-xylofuranosyl nucleosides (I; R = H, 9-adeninyl,
AR
     1-cytosinyl, 1-uracidlyl, 1-thyminyl, 9-(2-amino-6-chloropurinyl), etc.
     and R1 = H, 9-adeninyl, 1-cytosinyl, or 4-carbamoyl-5-aminoimidazolyl)
     were prepd. (.beta.-anomers by glycosylation of the purine and pyrimidine
     aglycons with 1-0-acetyl-2,3,5-tri-0-benzoyl-.alpha.-D-xylofuranose
     [20822-87-1] or 1,2-di-O-acetyl-3,5-di-O-benzoyl-.alpha.-D-xylofuranose
     [83434-58-6] followed by deblocking; .alpha.-anomers by multistep
     synthesis starting with the appropriate amino- or
     mercaptoxylofuranooxazolines) and tested for acute toxicity and
     therapeutic activity against herpetic encephalitis in mice, antiviral
     action in vitro, cytotoxicity to myeloma SP2 cells in suspension culture,
     and inhibitory activity against macromol. synthesis in rabbit kidney cells
     in primary culture. Three I, .beta.-D-xylofuranosyl nucleosides of
     adenine, guanine, and cytosine, showed marked biol. activity.
     xylofuranosyl nucleoside prepn biol activity; antiviral xylofuranosyl
ST
     nucleoside; antitumor xylofuranosyl nucleoside; toxicity xylofuranosyl
     xylofuranosyl nucleoside
ΙT
     Encephalitis
ΙT
     Deoxyribonucleic acid formation
     Protein formation
```

nucleoside; cytotoxicity xylofuranosyl nucleoside; macromol formation (from herpes virus, xylofuranosyl nucleosides treatment of)

Ribonucleic acid formation (inhibition of, by xylofuranosyl nucleosides)

ΙT Neoplasm inhibitors Virucides and Virustats

(xylofuranosyl nucleosides)

ΙT Toxicity

(acute, of xylofuranosyl nucleosides)

ΙT Nucleosides, preparation

RL: SPN (Synthetic preparation); PREP (Preparation) (xylofuranosyl, prepn. and neoplasm-inhibiting and antiviral and cytotoxic activities of)

ΙT 110-89-4, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (Mannich reaction of, with xylofuranosyluracil)

65-71-4 66-22-8, biological studies 71-30-7 73-24-5, biological IΤ studies 10310-21-1

RL: BIOL (Biological study)

(condensation of; with peracylated xylofuranoses)

TΤ 58-86-6, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(conversion of, to oxazoline)

ΙT 20822-87-1 83434-58-6

RL: BIOL (Biological study)

(glycosylation of purines and pyrimidines with)

```
ΙT
      99355-43-8P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
          (prepn. and amination of)
 IT
      99355-42-7P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and base-catalyzed cyclization and deprotection of)
 ΙT
      99436-42-7P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and conversion to oxazoline)
      77180-84-8P
 TΨ
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and conversion to thiouracil deriv.)
      99376-19-9P
 ΙT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and cyclization with triethylformate)
 TΤ
      99355-39-2P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. and deacetylation of)
 TΤ
      99355-37-0P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. and dehydration of)
 ΙT
      52448-07-4P
                    83373-05-1P 99355-30-3P
      99355-31-4P
                    99355-32-5P
                                  99355-33-6P
                                                 99355-40-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
      (Preparation); RACT (Reactant or reagent)
         (prepn. and deprotection of)
     99355-36-9P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and desilylation or acetylation of or reaction
        benzoylisothiocyanate)
IT
     99355-44-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and hydrogenolysis of)
     99355-41-6P
ΤŢ
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and methylation of)
ΙT
     58-86-6DP, purine and pyrmidine nucleosides
                                                    524-69-6P
                                                                2946-52-3P
     3530-56-1P 16535-78-7P
                              26017-62-9P
                                             27462-39-1P
     52486-19-8P
                   53294-14-7P 89618-08-6P
                                              99355-34-7P
     99436-41-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and neoplasm-inhibiting and antiviral and cytotoxic activities
        of)
ΙT
     41545-82-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and protection or Mannich reaction with piperidine)
ΙT
     41545-78-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction with Me propiolate)
IT
     99436-43-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction with aminocyanoacetamide or hydrolysis of)
     99355-38-1P
IΤ
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction with formamidine acetate or deacetylation of)
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41545-80-6P
 IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and ring-opening of)
      89595-52-8P
                    89596-51-0P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and substitution reaction with thiourea)
 ΙT
      27462-38-0P 77172-20-4P 99355-35-8P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
IT
      3473-63-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with [acetylbis(butyldimethylsilyl)xylofuranosyl]cyanoami
         noimidazole)
IT
     532-55-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with [bis(butyldimethylsilyl)xylofuranosyl]carbamoylamino
        imidazole)
ΤТ
     922-67-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with aminoxylofuranoxazoline)
     6719-21-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with bis(butyldimethylsilyl)xylofuranoxazoline)
IΤ
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (silylation of)
ፐጥ
     62-56-6, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (substitution reaction of, with aminochloropurine xylofuranosides)
IT
     122-51-0
     RL: BIOL (Biological study)
        (xylofuranosylcyanoaminoimidazole cyclization with)
IT
     77180-84-8P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and conversion to thiouracil deriv.)
RN
     77180-84-8 HCAPLUS
    2,4(1H,3H)-Pyrimidinedione, 1-(2,3,5-tri-O-benzoyl-.alpha.-D-
CN
     xylofuranosyl)- (9CI) (CA INDEX NAME)
```

RN 99355-30-3 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2,3,5-tri-O-benzoyl-.beta.-D-xylofuranosyl)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 99355-31-4 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-O-acetyl-3,5-di-O-benzoyl-.beta.-D-xylofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### IT 3530-56-1P 16535-78-7P 52486-19-8P

89618-08-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and neoplasm-inhibiting and antiviral and cytotoxic activities
 of)

RN 3530-56-1 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

RN 16535-78-7 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-.beta.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 52486-19-8 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-methyl-1-.beta.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 89618-08-6 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-methyl-1-.alpha.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

IT 41545-82-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and protection or Mannich reaction with piperidine)

RN 41545-82-8 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-.alpha.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 77172-20-4P

RN 77172-20-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.alpha.-D-xylofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1982:510325 HCAPLUS

DN 97:110325

TI 4-(1,2,4-Triazol-1-yl)- and 4-(3-nitro-1,2,4-triazol-1-yl)-1-(.beta.-D-2,3,5-tri-O-acetylarabinofuranosyl)pyrimidin-2(1H)-ones. Valuable intermediates in the synthesis of derivatives of 1-(.beta.-D-arabinofuranosyl)cytosine (ara-C)

AU Divakar, K. J.; Reese, Colin B.

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CS Dep. Chem., King's Coll., London, WC2R 2LS, UK

Journal of the Chemical Society, Perkin Transactions 1: Organic and
Bio-Organic Chemistry (1972-1999) (1982), (5), 1171-6

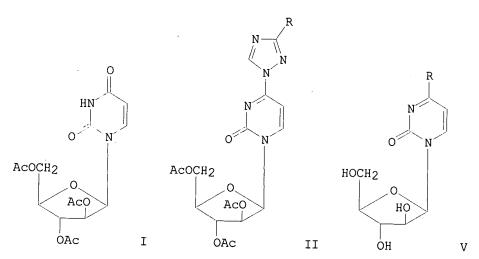
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

CC 33-9 (Carbohydrates)
Section cross-reference(s): 23, 25, 28

GI
```



(Preparation); RACT (Reactant or reagent)

Condensation reactions of triacetylarabinofuranosyluracil (I), prepd. in 3 AΒ steps from uracil, with tri(1H-1,2,4-triazol-1-yl)phosphine oxide and with 3-nitro-1,2,4-triazole and (PhO)2POC1 gave the title compds. II (R = H,NO2) (III and IV, resp.). Substitution reactions of III with RH (R = NH2, NHMe, NMe2, morpholino, PhNH, p-MeC6H4S) gave the corresponding arabinofuranosylcytosines V in high yield. Substitution of IV with PhNH2 and with H2NCH2CO2Me gave V (R = PhNH, NHCH2CO2Me, resp.). arabinofuranosyluracil prepn condensation triazole; ST triazolylarabinofuranosylpyrimidinone prepn substitution; cytosine arabinofuranosyl ΙT Nucleosides, preparation RL: SPN (Synthetic preparation); PREP (Preparation) (arabinofuranosylcytosines, prepn. of, by substitution reactions of triazolyl(triacetylarabinofuranosyl)pyrimidinones with amines TΤ Substitution reaction, nucleophilic (of triazolyl(triacetylarabinofuranosyl)pyrimidinones, with amines and with toluenethiol) 24807-55-4 ΙT 72741-18-5 RL: RCT (Reactant); RACT (Reactant or reagent) (condensation reaction of, with (triacetylarabinofuranosyl)uracil) IT 66-22-8, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (cyclocondensation reaction of, intramol.) IT 3083-77-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and acetylation of) 14057-18-2P ΙT RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(prepn. and condensation reactions of, with tritriazolylphosphine oxide

and nitrotriazole) ΙT 3736-77-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and hydrolysis of) ΙT 82855-62-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and substitution reactions of, with amines and with toluenethiol) IT 82855-63-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and substitution reactions of, with aniline and with glycine Me ester) ΙT 147-94-4P 13491-42-4P 82855-64-9P **82855-65-0P 82855-66-1P** 82855-67-2P 82855-68-3P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 74-89-5, reactions 106-45-6 110-91-8, reactions 124-40-3, reactions 616-34-2 7664-41-7, reactions IT RL: RCT (Reactant); RACT (Reactant or reagent) (substitution reaction of, with triazolyl[triacetylarabinofuranosyl)pyr imidinone) ΙT 62-53-3, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (substitution reactions of, with triazolyl(triacetylarabinofuranosyl)py rimidinones) IT 3083-77-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

2,4(1H,3H)-Pyrimidinedione, 1-.beta.-D-arabinofuranosyl- (9CI) (CA INDEX

Absolute stereochemistry.

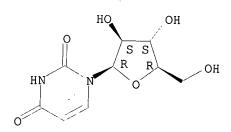
NAME)

3083-77-0 HCAPLUS

RN

CN

(prepn. and acetylation of)



#### IT 14057-18-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and condensation reactions of, with tritriazolylphosphine oxide and nitrotriazole)

14057-18-2 HCAPLUS RN

2,4(1H,3H)-Pyrimidinedione, 1-(2,3,5-tri-O-acetyl-.beta.-D-CN arabinofuranosyl) - (9CI) (CA INDEX NAME)

#### IT 82855-62-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and substitution reactions of, with amines and with toluenethiol)

RN 82855-62-7 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-(2,3,5-tri-O-acetyl-.beta.-D-arabinofuranosyl)-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 82855-63-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and substitution reactions of, with aniline and with glycine Me ester)

RN 82855-63-8 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(3-nitro-1H-1,2,4-triazol-1-yl)-1-(2,3,5-tri-0-acetyl-.beta.-D-arabinofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# IT 147-94-4P 13491-42-4P 82855-64-9P 82855-65-0P 82855-66-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 147-94-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 13491-42-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-.beta.-D-arabinofuranosyl-4-(methylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 82855-64-9 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-.beta.-D-arabinofuranosyl-4-(dimethylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 82855-65-0 HCAPLUS

CN 2(1H)-Pyrimidinone, 1-.beta.-D-arabinofuranosyl-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

RN 82855-66-1 HCAPLUS

2(1H)-Pyrimidinone, 1-.beta.-D-arabinofuranosyl-4-(phenylamino)- (9CI) CN (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2003 ACS

ΑN 1981:121849 HCAPLUS

DN 94:121849

ΤI Methylation study of ribonucleosides, deoxyribonucleosides, and 2'-O-methylribonucleosides with trimethylsulfonium hydroxide and trimethylsulfonium iodide. Influence of the 2'-hydroxy-groups on the reactivity of the base moieties of ribonucleosides

Yamauchi, Kiyoshi; Nakagima, Toru; Kinoshita, Masayoshi Dep. Appl. Chem., Osaka City Univ., Osaka, 558, Japan ΑU

CS

Journal of the Chemical Society, Perkin Transactions 1: Organic and SO Bio-Organic Chemistry (1972-1999) (1980), (12), 2787-92 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

CC 33-7 (Carbohydrates)

Section cross-reference(s): 22

The methylation reactions were examd. of the nucleosides adenosine (I), AΒ guanosine (II), cytidine (III), uridine (IV), and inosine, the deoxy derivs. of I, II, III, IV, and thymidine, and the 2'-0-Me derivs. of I, III, and IV with Me3SOH and Me3SI (DMF, 70-85.degree., 1-3.5 h). The deoxy and 2'-O-Me derivs. showed very similar behavior both in reactivity of the base moiety and in the methylation pattern, but the nucleosides had a much less reactive base group and gave different methylation products. The reactivities are discussed in terms of intramol. H-bonding between the 2'-OH and amine groups. The methylating characteristics of Me3SOH and Me3SI are also described. Kinetic studies indicated an SN2 mechanism for methylation of nucleosides by Me3S+ ion. ST

nucleoside methylation trimethylsulfonium kinetics; ribonucleoside methylation trimethylsulfonium kinetics; deoxyribonucleoside methylation trimethylsulfonium kinetics; methylribonucleoside methylation trimethylsulfonium kinetics; methylsulfonium methylation ribonucleoside

```
kinetics; hydrogen bond nucleoside methylation
  ΙT
       Kinetics of methylation
      Methylation
          (of ribonucleosides by trimethylsulfonium ion)
  IT
      Nucleosides, reactions
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (deoxyribo-, methylation of, by trimethylsulfonium ion, kinetics of)
      Nucleosides, reactions
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (ribo-, methylation of, by trimethylsulfonium ion, kinetics of)
 IT
      2181-42-2
                   17287-03-5
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (methylation by, of ribonucleosides, kinetics of)
 TΤ
      50-89-5, reactions 58-61-7, reactions 58-63-9 58-96-8
      65-46-3
               118-00-3, reactions 951-77-9 951-78-0
      958-09-8
                 961-07-9 2140-72-9 2140-76-3
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (methylation of, by trimethylsulfonium ion, kinetics of)
 TΤ
      76551-26-3P
                    76551-27-4P
                                   76551-28-5P
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of)
 IT
      1867-73-8P
                   10300-22-8P
                                  15763-06-1P
                                                60037-52-7P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of adenosine)
 IT
      57817-83-1P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of adenosine and methyladenosine) 94-00-7P 76567-64-1P
 ΙT
      20594-00-7P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of cytidine)
ΙT
      2002-35-9P
                   3413-67-0P
                                35665-58-8P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of deoxyadenosine)
IT
      22882-02-6P
                   76551-25-2P
                                  76567-65-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of deoxycytidine)
IT
      5132-79-6P
                   26718-69-4P
                                 76551-22-9P
                                                76551-23-0P
                                                              76551-24-1P
      76567-63-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of deoxyguanosine)
     958-74-7P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, by methylation of deoxythymidine)
TΤ
     24514-32-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by methylation of deoxyuridine)
IT
     2140-65-0P
                  2140-71-8P
                                10300-27-3P
                                              15313-37-8P
                                                             73667-71-7P
     74466-66-3P
                   76551-21-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by methylation of guanosine)
TΨ
     2140-73-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by methylation of inosine)
IT
     20649-46-1P
                   30891-53-3P
                                 76567-62-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by methylation of methyladenosine)
ΙT
     13048-95-8P
                   34218-86-5P
                                 76567-66-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by methylation of methylcytidine)
IT
     7103-27-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, by methylation of methyluridine)
ΙT
     2140-69-4P
```

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by methylation of uridine)

IT 50-89-5, reactions 58-96-8 65-46-3 951-77-9 951-78-0 2140-72-9 2140-76-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(methylation of, by trimethylsulfonium ion, kinetics of)

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 58-96-8 HCAPLUS CN Uridine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 65-46-3 HCAPLUS CN Cytidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 951-77-9 HCAPLUS
CN Cytidine, 2'-deoxy- (80

Cytidine, 2'-deoxy- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 951-78-0 HCAPLUS CN Uridine, 2'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 2140-72-9 HCAPLUS CN Cytidine, 2'-O-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 2140-76-3 HCAPLUS CN Uridine, 2'-O-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### IT 22882-02-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by methylation of deoxycytidine)

RN 22882-02-6 HCAPLUS

Cytidine, 2'-deoxy-N-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

ΙT 13048-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by methylation of methylcytidine) 13048-95-8 HCAPLUS

RN

Cytidine, N-methyl-2'-O-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2003 ACS L75

ΑN 1980:592052 HCAPLUS

DN 93:192052

Antiviral composition and method of treating virus diseases ΤI

ΙN Greer, Sheldon

University of Miami, USA; PCR Inc. PΑ

SO U.S., 11 pp. CODEN: USXXAM

DTPatent

LA English

IC A61K031-70; C07H017-00

NCL 424180000

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 3, 33

FAN.CN	2 2					
P.F.	ATENT NO.	KIND	DATE		APPLICATION NO.	DATE
GE DE DE GE GE PRAI US	4210638 1588550 2838644 2838644 2021097 1978-887541	A A A1 C2 A B2	19800701 19810423 19790927 19890202 19791128 19821006 19780317	<	US 1978-887541 GB 1978-24858 DE 1978-2838644 GB 1979-9319	19780317 < 19780531 < 19780905 < 19790316 <
	1978-887555		19780317	<		
GI	1978-887745		19780317	<		

A combination of 5-trifluoromethyl-2'-deoxycytidine (I) AB 66384-66-5] and a cytidine deaminase inhibitor, such as tetrahydrouridine [18771-50-1] or 2'-deoxytetrahydrouridine [31962-88-6] is an effective virucide, esp. for Herpes simplex. I was prepd. by treating 5-trifluoromethyl-2'-deoxyuridine [70-00-8], in which the free hydroxy groups have been protected (silylated), with NH3. virucide trifluoromethyldeoxycytidine; tetrahydrouridine trifluoromethyldeoxycytidine virucide ΙT Virucides and Virustats (trifluoromethyldeoxycytidine-cytidine deaminase inhibitor compns.) IT 70-00-8 RL: RCT (Reactant); RACT (Reactant or reagent) (amination of, in trifluoromethyldeoxycytidine virucide prepn.) IT 66384-66-5P RL: PREP (Preparation) (prepn. and virucidal compns. contg. cytidine deaminase inhibitor and) ΙT 18771-50-1 31962-88-6 RL: BIOL (Biological study) (virucidal compns. contg. trifluoromethyldeoxycytidine and) ΙT 70-00-8 RL: RCT (Reactant); RACT (Reactant or reagent) (amination of, in trifluoromethyldeoxycytidine virucide prepn.) RN 70-00-8 HCAPLUS Thymidine, .alpha.,.alpha.,trifluoro- (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

#### IT 66384-66-5P

RN

CN

RL: PREP (Preparation)
 (prepn. and virucidal compns. contg. cytidine deaminase inhibitor and)
66384-66-5 HCAPLUS
Cytidine, 2'-deoxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2003 ACS

ΑN 1980:129265 HCAPLUS

DN 92:129265

TI 5-Trifluoromethyl-2'-deoxycytidine

Greer, Sheldon B.; Stump, Eugene G., Jr.; Psarras, Theodore IN

PΑ PCR Inc., USA; University of Miami

SO Ger. Offen., 42 pp.

CODEN: GWXXBX

DT Patent

LA German

IC C07H019-06

CC 33-7 (Carbohydrates)

Section cross-reference(s): 63

FAN.CNT 2

I AIV.	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
ΡI	DE 2838644 DE 2838644	A1 C2	19790927 19890202		DE 1978-2838644	19780905 <
PRAI GI	US 4210638 JP 54128587 US 1978-887541 US 1978-887555 US 1978-887745	A A2	19800701 19791005 19780317 19780317 19780317	< <	US 1978-887541 JP 1978-109549	19780317 < 19780906 <

AΒ Title compd. I was prepd. by silylation of 5-trifluoromethyl-2'-deoxyuridine with HN(SiMe3)2 followed by treatment with NH3-NH4Cl. I is virucidal against Herpes viruses and in the presence of a cytidine deaminase inhibitor has a lower cytotoxicity and greater stability than known compds., such as trifluorothymidine.

ST fluoromethyldeoxycytidine; deoxycytidine trifluoromethyl; virucide trifluoromethyldeoxycytidine

IT Virucides and Virustats

(trifluorodeoxycytidine)

IT 66384-66-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and virucidal activity of)

IT 70-00-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(silylation and amination of)

IT 66384-66-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and virucidal activity of)

RN 66384-66-5 HCAPLUS

CN Cytidine, 2'-deoxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 70-00-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(silylation and amination of)

RN 70-00-8 HCAPLUS

CN Thymidine, .alpha.,.alpha.-trifluoro- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1979:413506 HCAPLUS

DN 91:13506

TI Synthesis and antiviral activities of arabinofuranosyl-5-ethylpyrimidine nucleosides. Selective antiherpes activity of 1-(.beta.-D-arabinofuranosyl)-5-ethyluracil

AU Kulikowski, Tadeusz; Zawadzki, Zbigniew; Shugar, David; Descamps, Johan; De Clercq, Erik

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CS Inst. Biochem. Biophys., Pol. Acad. Sci., Warsaw, Pol. So Journal of Medicinal Chemistry (1979), 22(6), 647-53 CODEN: JMCMAR; ISSN: 0022-2623 Journal LA English CC 1-4 (Pharmacodynamics) Section cross-reference(s): 33
```

Ι

```
Arabinofuranosyl-5-ethylpyrinidine nucleosides were prepd. by several
AΒ
     procedures and their activities tested in primary rabbit kidney cells and
      in human skin fibroblasts. 1-.beta.-D-Arabinsfuranosyl-5-ethyluracil (I) [70020-72-3], prepd. by the condensation of 2,3,5-tri-O-(benzyl)-
      .alpha.-D-arabinofuranosyl chloride [4060-34-8] with 2,4-bis-0-
      (trimethylsilyl)-5-ethyluracil [10457-14-4] in ClCH2CH2Cl in the presence
     of mol. sieves or SnCl4, inhibited herpes simplex virus at a concn. as low
     as 2 ug/mL. The .alpha.-anomer of I was inactive. CD and NMR data are
     given.
ST
     pyrimidine nucleoside prepn virucide
ΙT
     Virucides and Virustats
         (arabinsfuranosylethylpyrimidine nucleosides)
ΙT
     Circular dichroism
     Nuclear magnetic resonance
         (of arabinofuranosylethylpyrinidine nucleosides)
ΙT
     Chromatography, thin-layer
         (of arabinsfuranosylethylpyrimidine nucleosides)
ΙT
     4060-34-8
     RL: BIOL (Biological study)
        (condensation of, with bis(trimethylsilyl)ethyluracil)
IT
     70051-90-0
     RL: BIOL (Biological study)
        (condensation of, with bis(trimethylsilyl)ethyluriacil)
ΙT
     52492-40-7
     RL: BIOL (Biological study)
         (condensation of, with diethoxyethylpyrimidine)
     34171-35-2
     RL: BIOL (Biological study)
        (condensation of, with tribenzylarabinofuranosyl bromide)
IΤ
     999-97-3
     RL: BIOL (Biological study)
        (ethyluracil silyation by)
IΤ
     70020-81-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and amination and hydrolysis of)
IT
     70020-79-0P
                    70020-80-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
```

```
(Reactant or reagent)
         (prepn. and amination of)
IT
      10457-14-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and condensation of, with arabinosfuranose- and uracil derivs.)
ΙT
     70020-77-8P 70020-78-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
         (prepn. and reaction with phosphorus pentasulfide)
     70020-76-7P
ΙT
                   70020-82-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and redn. of)
IT
     70020-72-3P 70020-73-4P 70020-74-5P
     70020-75-6P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. and virucidal activity of)
     4348-68-9
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with bis(trimethylsilyl)ethyluracil)
     4212-49-1
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (silylation of)
     70020-77-8P 70020-78-9P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (prepn. and reaction with phosphorus pentasulfide)
     70020-77-8 HCAPLUS
RN
    2,4(1H,3H)-Pyrimidinedione, 5-ethyl-1-(2,3,5-tri-O-benzoyl-.alpha.-D-
CN
     arabinofuranosyl) - (9CI) (CA INDEX NAME)
```

RN 70020-78-9 HCAPLUS CN

2,4(1H,3H)-Pyrimidinedione, 5-ethyl-1-(2,3,5-tri-O-benzoyl-.beta.-Darabinofuranosyl) - (9CI) (CA INDEX NAME)

## TT 70020-72-3P 70020-73-4P 70020-74-5P 70020-75-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and virucidal activity of)

RN 70020-72-3 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-.beta.-D-arabinofuranosyl-5-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 70020-73-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl-5-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 70020-74-5 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-.alpha.-D-arabinofuranosyl-5-ethyl- (9CI) (CA INDEX NAME)

RN 70020-75-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.alpha.-D-arabinofuranosyl-5-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1979:413469 HCAPLUS

DN 91:13469

TI Design of species- or isozyme-specific enzyme inhibitors. I. Effect of thymidine substituents on affinity for the thymidine site of hamster cytoplasmic thymidine kinase

AU Hampton, Alexander; Kappler, Francis; Chawla, Ram R.

CS Fox Chase Cancer Cent., Inst. Cancer Res., Philadelphia, PA, 19111, USA

Journal of Medicinal Chemistry (1979), 22(6), 621-31 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

CC 1-3 (Pharmacodynamics)

Section cross-reference(s): 7, 33

GΙ

```
5-(Ethylamino)-2'-deoxyuridine (I) [5155-07-7] was a very weak inhibitor
 AB
      of hamster thymidine kinase [9002-06-6] and longer-chain
      5-(acylamino)-2'-deoxyuridines were weak noncompetitive inhibitors.
                                                                             The
      above, their phosphates and some of their analogs were synthesized.
                                                                             The
      concn. dependence of their inhibitory action on the enzyme resembled that
      of the feedback inhibitor TTP. Enzyme-inhibitor dissocn. consts. (Ki
      values) were detd. for thymidine derivs. monosubstituted at various
      positions. There is evidence that attachment of suitable substituents to
      thymidine could, in principle, lead to thymidine site directed
      isoenzyme-specific inhibitors of human cytoplasmic thymidine kinase, which
      is a candidate target in the design of antineoplastic drugs.
 ST
      deoxyuridine deriv thymidine kinase inhibitor
 IT
      Kinetics, enzymic
         (of inhibition, of thymidine kinase)
 ΙT
      16357-59-8
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (acylation by, of nucleosides)
IT
      5536-30-1
                  25152-20-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (acylation of, by (ethoxycarbonyl)ethoxydihydroquinoline)
     9002-06-6
ΙT
     RL: PROC (Process)
         (inhibition of, by deoxythymidines and deoxyuridines)
ΙT
     70465-57-5P
                   70465-58-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and conversion triphosphate)
ΙT
     70465-91-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and isolation of)
IT.
     5155-07-7P
                  5536-30-1P
                                             21473-40-5P
                                7236-56-8P
                                                           21888-81-3P
     26639-00-9P
                   52450-18-7P
                                  63614-47-1P
                                                70465-51-9P
                                                              70465-52-0P
     70465-53-1P
                   70465-54-2P
                                  70465-55-3P
                                                70465-56-4P
                                                              70465-59-7P
     70465-60-0P 70465-61-1P
                               70465-62-2P
                                              70465-63-3P
     70465-64-4P
                   70465-65-5P
                                  70465-66-6P
                                                70465-67-7P
                                                              70465-68-8P
     70465-69-9P
                   70465-70-2P
                                  70465-72-4P
                                                70465-73-5P
                                                              70465-74-6P
     70465-75-7P
                   70465-76-8P
                                  70465-77-9P
                                                70465-78-0P
                                                              70465-79-1P
     70465-80-4P
                   70465-81-5P
                                  70465-82-6P
                                                70465-83-7P
                                                              70465-84-8P
     70465-85-9P
                   70465-86-0P
                                  70575-53-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and thymidine kinase-inhibiting activity of)
     70465-71-3P
IT
                   70465-87-1P
                                 70465-88-2P
                                                70465-89-3P
                                                              70465-90-6P
                   70491-64-4P
     70465-92-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
ΙT
     7253-19-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with alkylamines)
```

ΙT 1763-02-6

> RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with amines)

IT 54-42-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with amines and with potassium cyanate)

70465-93-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with ethanethiol)

IΤ 64966-96-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with ethylamine)

ΙT 110-70-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with tosylthymidine)

IT53435-03-3 53495-39-9 70465-94-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)

(thymidine kinase-inhibiting activity of)

IT 70465-61-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and thymidine kinase-inhibiting activity of)

70465-61-1 HCAPLUS RN

Cytidine, 2'-deoxy-N-ethyl- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

ΙT 54-42-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with amines and with potassium cyanate)

RN 54-42-2 HCAPLUS

Uridine, 2'-deoxy-5-iodo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry. Rotation (+).

ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2003 ACS L75

ΑN 1979:87784 HCAPLUS

DN 90:87784

```
The synthesis of nucleosides derived from 5-ethynyluracil and
TI
     5-ethynylcytosine
```

Barr, Philip J.; Jones, A. Stanley; Serafinowski, Pawel; Walker, Richard ΑU

CS Chem. Dep., Univ. Birmingham, Birmingham, UK

Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (10), 1263-7 CODEN: JCPRB4; ISSN: 0300-922X

DΤ Journal LA English

33-7 (Carbohydrates) CC

GI

$$C\equiv CH$$
 $C=CH_2$ 
 $C=CH_2$ 
 $C=CH_2$ 

5-Ethynyluridine, 2'-deoxy-5-ethynyluridine, and its .alpha.-anomer (I; R = H, R1R2 = O, R3 = .beta.-D-ribofuranosyl, 2-deoxy-.beta.-D-erythro-AΒ pentofuranosyl, -.alpha.-D-erythro-pentofuranosyl, resp.) were prepd. by condensation of the trimethylsilyl deriv. of 5-ethynyluracil (I; R = R3 = H, R1R2 = 0) with the appropriate blocked sugar derivs. and removal of the blocking groups. Treatment of the pyrimidine II (R = R1 = C1) with NH3 gave a mixt. of II [R = NH2, R1 = C1; R = C1, R1 = NH2 (III)]; treatment of III with KOH in aq. dioxane gave 5-ethynylcytosine (I; RR1 = bond, R2 = NH2, R3 = H) (IV). Condensation of the trimethylsilyl deriv. of IV with the appropriate protected sugar derivs. and removal of the protecting groups gave 5-ethynylcytidine, 2'-deoxy-5-ethynylcytidine, and its .alpha.-anomer (I; RR1 = bond, R2 = NH2, R3 = .beta.-D-ribofuranosyl, 2-deoxy-.beta.-D-erythro-pentofuranosyl, -.alpha.-D-erythropentofuranosyl, resp.).

uridine ethynyl; cytosine ethynyl; cytidine ethynyl; ethynyl nucleoside STIT

Nucleosides, preparation

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from ethynyluracil and -cytosine)

ΙT 61751-45-9

RL: RCT (Reactant); RACT (Reactant or reagent) (amination of)

ΙT 4330-21-6 6974-32-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation reaction of, with bis(trimethylsilyl) deriv. of ethynyluracil)

69075-40-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and condensation reaction of, with acetyltribenzoylribofuranose and chlorodeoxyditoluoylpentofuranose)

TΨ 65223-79-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and conversion of, to etynylcytidine)

65223-81-6P 69075-41-8P ΙT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. and debenzoylation of) IT 69075-43-0P 69075-44-1P 69075-45-2P 69075-46-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and detoluoylation of) ΙT 65223-77-0P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) ΙT 65223-78-1P 69075-47-4P 69275-22-5P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from ethynylcytosine) IT 61135-33-9P 69075-42-9P 69101-77-5P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from ethynyluracil) 65223-82-7P ΙT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn., oxidn., and dehydrochlorination of) ΙT 59989-18-3 RL: RCT (Reactant); RACT (Reactant or reagent) (trimethylsilylation of) ΙT 65223-81-6P 69075-41-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and debenzoylation of) RN 65223-81-6 HCAPLUS Cytidine, 5-ethynyl-, 2',3',5'-tribenzoate (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN 69075-41-8 HCAPLUS CN Uridine, 5-ethynyl-, 2',3',5'-tribenzoate (9CI) (CA INDEX NAME)

### 69075-46-3P

RN 69075-43-0 HCAPLUS

CN Uridine, 2'-deoxy-5-ethynyl-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 69075-44-1 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-.alpha.-D-erythro-pentofuranosyl]-5-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 69075-45-2 HCAPLUS

CN Cytidine, 2'-deoxy-5-ethynyl-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

RN 69075-46-3 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-.alpha.-D-erythro-pentofuranosyl]-5-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$HC = C$$
 $H_2N$ 
 $N$ 
 $N$ 
 $S$ 
 $R$ 
 $O$ 
 $Me$ 

## IT 65223-78-1P 69075-47-4P 69275-22-5P

RN 65223-78-1 HCAPLUS

CN Cytidine, 5-ethynyl- (9CI) (CA INDEX NAME)

RN 69075-47-4 HCAPLUS CN Cytidine, 2'-deoxy-5-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 69275-22-5 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-.alpha.-D-erythro-pentofuranosyl)-5-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 61135-33-9P 69075-42-9P 69101-77-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from ethynyluracil)

RN 61135-33-9 HCAPLUS

CN Uridine, 2'-deoxy-5-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 69075-42-9 HCAPLUS CN Uridine, 5-ethynyl- (9CI) (CA INDEX NAME)

RN 69101-77-5 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-.alpha.-D-erythro-pentofuranosyl)-5-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2003 ACS

AN 1977:106946 HCAPLUS

DN 86:106946

TI Transformation of 5-(polyfluoroalkyl)- and 5-(polyfluoroalkoxymethyl)uridines

AU Mel'nik, S. Ya.; Bakhmedova, A. A.; Sof'in, A. V.; Vornovitskaya, G.I.; Dubinina, I. G.; Preobrazhenskaya, M. N.

CS Cancer Res. Cent., Moscow, USSR

SO Bioorganicheskaya Khimiya (1976), 2(11), 1520-5 CODEN: BIKHD7; ISSN: 0132-3423

DT Journal

LA Russian

CC 33-7 (Carbohydrates)

Section cross-reference(s): 28

GΙ

## \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Cyclization of 5-(3,3,3-trifluoropropyl) uridine by (PhO)2CO gave 56% 2,2'-anhydro deriv. which was cleaved by base to give 76% I (R = H, X = O). The latter was acetylated and treated with P2S5 to give 88% I (R = Ac, X = S) which was aminated to give 57% II. Acetylation of III (R = H, X = O) followed by treatment with P2S5 gave 52.3% III (R = Ac, III (R = H, X = O), and 5-(3,3,3-trifluoroethoxymethyl) uridine had no effect on uridinekinase, UMP-, and UdP-kinases in enzyme systems

```
phosphorylating uridine to UMP or UMP to UTP.
      uridine polyfluoroalkyl; fluoroalkoxyuridine; polyfluoroalkoxymethyl
 ST
      uridine
 IT
      102-09-0
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclization of trifluoropropyluridine by)
      55420-09-2
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclization of, by diphenyl carbonate)
 ΙT
      9026-39-5
                  9026-51-1
                              9036-23-1
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (effect of polyfluoroalkyl- and polyfluoroalkoxymethyluridines on)
 ΙT
      62012-59-3P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP
      (Preparation); RACT (Reactant or reagent)
         (prepn. and acetylation of)
 ΙT
      59694-34-7P
                    59727-26-3P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and effect on uridine kinase)
IΤ
      62012-61-7P
                    62012-63-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. and reaction with ammonia)
IT
     59694-33-6P 62012-60-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
         (prepn. and reaction with phosphorus pentasulfide)
ΙT
     62042-31-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and ring cleavage of)
ΙT
     62012-62-8P
                  62012-64-0P
                                  62012-65-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
ΙT
     55420-09-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclization of, by diphenyl carbonate)
RN
     55420-09-2 HCAPLUS
     Uridine, 5-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)
CN
Absolute stereochemistry.
```

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ΙT
      62012-59-3P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
         (prepn. and acetylation of)
RN
      62012-59-3 HCAPLUS
      2,4(1H,3H)-Pyrimidinedione, 1-.beta.-D-arabinofuranosyl-5-(3,3,3-
CN
      trifluoropropyl) - (9CI) (CA INDEX NAME)
```

IT 62012-60-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction with phosphorus pentasulfide)

RN 62012-60-6 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-(2,3,5-tri-O-acetyl-.beta.-D-arabinofuranosyl)-1-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 62012-62-8P

RN 62012-62-8 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-arabinofuranosyl-5-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L75 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2003 ACS AN 1975:497822 HCAPLUS

RN 5241-10-1 HCAPLUS

CN Cytidine, 2'-deoxy-5-methyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 18839-89-9 HCAPLUS CN Cytidine, N-phenyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 29834-86-4 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-(1-pyrrolidinyl)-1-.beta.-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

RN 39824-59-4 HCAPLUS CN 2(1H)-Pyrimidinone, 4-(4-morpholinyl)-1-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 50-89-5, reactions 58-96-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (silylation and amination of)

RN 50-89-5 HCAPLUS

CN Thymidine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 58-96-8 HCAPLUS CN Uridine (8CI, 9CI) (CA INDEX NAME)

```
DN
      83:97822
      Syntheses of nucleosides. XIV. Amination of heterocycles.
 ΤI
      New simple synthesis of cytidines
      Vorbrueggen, Helmut; Krolikiewicz, Konrad; Niedballa, Ulrich
 ΑU
      Forschungslab., Schering A.-G., Berlin, Fed. Rep. Ger.
 CS
      Justus Liebigs Annalen der Chemie (1975), (5), 988-1002
 SO
      CODEN: JLACBF; ISSN: 0075-4617
 DT
      Journal
 LΑ
      German
 CC
      33-7 (Carbohydrates)
      Cytidines were prepd. by persilylation of free or acetylated uridines or
 AΒ
      uridine 5'-phosphates of the OH groups of the sugar moiety and the
      phosphate group followed by treatment with NH3 or primary or secondary
      amines. Thus, uridine reacted with (Me3Si) 2NH and NH3 in an
      autoclave for 0.5 hr at 24.degree. and 16 atm and 48 hr at 162.degree. and
      26 atm to give 72.5% cytidine.
      silylation amination uridine phosphate; cytidylic acid analog;
 ST
     cytosine deoxyribofuranosyl; cytidine; phenethylcytosine
     deoxyribofuranosyl; phenylcytidine deoxyribofuranosyl; azauridine
     pyrrolidinoribofuranosyl; thymidine amination
 IT
      75-12-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (amination of silylated nucleosides with)
IT
      62-53-3, reactions
                          64-04-0
                                     100-46-9
                                              108-00-9 110-91-8
                                                                      123-75-1
     7664-41-7, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (amination of silylated uridines with)
ΙT
     65-46-3P 5241-10-1P 18839-89-9P
     29834-86-4P
                   34948-48-6P
                                  35003-10-2P 39824-59-4P
     56982-72-0P
                   56982-73-1P
                                 56982-74-2P
                                              56982-75-3P
                                                              56982-77-5P
     56982-78-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
ΙT
     57025-16-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with ribose derivs.)
ΙT
     5991-01-5
                 6974-32-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with silylated triazines)
     50-89-5, reactions
ΙT
                          54-25-1 58-96-8
                                           1627-29-8
     3387-36-8
                 56982-76-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (silylation and amination of)
IT
     999-97-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (silylation of uridine derivs. with)
ΙT
     65-46-3P 5241-10-1P 18839-89-9P
     29834-86-4P 39824-59-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     65-46-3 HCAPLUS
     Cytidine (8CI, 9CI) (CA INDEX NAME)
```

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ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2003 ACS
 ΑN
      1974:421580 HCAPLUS
 DN
      81:21580
 TI
      5-Alkylpyrimidine nucleosides. Preparation and properties of
      5-ethyl-2'-deoxycytidine and related nucleosides
ΑU
      Kulikowski, T.; Shugar, D.
CS
      Inst. Biochem. Biophys., Acad. Sci., Warsaw, Pol.
SO
      Journal of Medicinal Chemistry (1974), 17(3), 269-73
      CODEN: JMCMAR; ISSN: 0022-2623
DT
      Journal
LA
     English
     3-2 (Biochemical Interactions)
CC
     Section cross-reference(s): 33
     5-Ethyl-2'-deoxycytidine (I) [50356-36-0] and its anomer
     1-(2-deoxy-.alpha.-D-ribofuranosyl)-5-ethylcytosine (II) [
     50499-40-6] were prepd. by thiation of .alpha.,.beta.-1-(3,5-di-O-
     p-chlorobenzoyl-2-D-ribofuranosyl)-5-ethyluracil with P2S5, thin-layer
     chromatog. sepn. of anomers, deblocking by treatment with NaOMe, and
     amination with NH3-MeOH. I had significant activity against
     herpes simplex virus, while 5'-phosphate esters of both I and II were
     dephosphorylated at comparable rates by snake venom 5'-nucleotidase
     [9027-73-0].
     cytidine ethyl deoxy antiviral; nucleotide dephosphorylation nucleotidase;
ST
     nucleoside cytidine antiviral
ΙT
     Dephosphorylation, biological
        (by nucleotidase, of ethyldeoxycytidine phosphate)
IT
     Virus, animal
        (herpes simplex, ethyldeoxycytidine inhibition of)
ΙT
     Circular dichroism
        (of 5-ethyl-2'-deoxynucleosides, conformation in relation to)
     Chromatography, thin-layer
ΙT
        (of 5-ethylpyrimidine 2'-deoxynucleosides, stereoisomer sepn. by)
IT
     9001-78-9
                 9027-73-0
     RL: PRP (Properties)
        (deoxycytidine 5'-phosphate dephosphorylation by)
TΨ
     52239-74-4
                 52239-75-5
     RL: PRP (Properties)
        (dephosphorylation of)
IT
     50356-36-0P 50499-40-6P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (prepn. and antiviral activity of)
ΙT
     52239-69-7P
                   52239-70-0P
                                 52239-71-1P 52239-72-2P
    52239-73-3P
                   52365-58-9P
                                 52365-59-0P
    RL: PREP (Preparation)
        (prepn. of)
ΙT
    75-77-4
               52304-86-6
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with cytosine deriv.)
```

IT 25137-84-2 25253-75-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(thiation of)

IT 32550-24-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(trimethylsilylation of)

IT 50356-36-0P 50499-40-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and antiviral activity of)

RN 50356-36-0 HCAPLUS

CN Cytidine, 2'-deoxy-5-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 50499-40-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-.alpha.-D-erythro-pentofuranosyl)-5-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 52239-72-2P 52239-73-3P

RN 52239-72-2 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-.alpha.-D-erythro-pentofuranosyl]-5-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{H}_2\text{N} \\ \text{N} \\ \text{O} \\ \text{S} \\ \text{R} \\ \text{O} \\ \text{Me} \\ \end{array}$$

RN 52239-73-3 HCAPLUS

CN Cytidine, 2'-deoxy-5-ethyl-, 3',5'-bis(4-methylbenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} \text{Et} \\ \text{H}_2\text{N} \\ \text{N} \\$$

IT 25137-84-2 25253-75-2

RL: RCT (Reactant); RACT (Reactant or reagent) (thiation of)

RN 25137-84-2 HCAPLUS

CN Uridine, 2'-deoxy-5-ethyl-, 3',5'-bis(4-chlorobenzoate) (9CI) (CA INDEX NAME)

RN

25253-75-2 HCAPLUS
2,4(1H,3H)-Pyrimidinedione, 1-[3,5-bis-O-(4-chlorobenzoyl)-2-deoxy-.alpha.-D-erythro-pentofuranosyl]-5-ethyl- (9CI) (CA INDEX NAME) CN